Monte Carlo and Series Expansion Studies of the Anisotropic Driven Ising Lattice Gas Phase Diagram

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(ABSTRACT)

While the statistical mechanics of systems in thermal equilibrium is a well established discipline, nonequilibrium systems are fundamentally much less well understood, even though most natural phenomena fall into the latter category. In particular, there is as yet no nonequilibrium analog for the systematic formalism of Gibbs ensembles. Rather than deal with the difficult problem of general nonequilibrium systems, this study is restricted to the steady states of a simple model whose equilibrium properties are well known.

The Ising lattice gas displays a number of surprising phenomena when driven into nonequilibrium steady states. This study extends previous work to a more general model with anisotropic interparticle interactions. Using Monte Carlo simulations, we obtain the phase diagram for the model, controlled by the driving field, temperature, and anisotropy parameter $\alpha \equiv \sqrt{\frac{\lambda}{T}}$. Under saturation drive, the shift in the transition temperature between ordered and disordered states can be either positive or negative, depending on $\alpha$. The possible existence at large $\alpha$ of an additional phase ordered in only one direction is discussed. For finite drives, both first and second order transitions are observed. A novel technique for locating the first order transition line is presented.

Some aspects of the phase diagram can be predicted by investigating the two-point correlation function to first order in a high temperature series expansion. However, the series expansion fails to predict even qualitatively the $\alpha$-dependence of the critical temperature.
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Chapter 1

Introduction

1.1 Background and Motivation

Understanding of systems of many particles in thermal equilibrium has improved greatly since the initial development of equilibrium statistical mechanics about a century ago. However, a similar theoretical framework to describe systems out of equilibrium does not yet exist. Physicists’ intuition about nonequilibrium systems is often flawed or incomplete. Because the majority of natural phenomena occur out of equilibrium, a theory to predict the behavior of such systems would certainly be desirable.

One approach toward understanding nonequilibrium systems is to study simple models. Though a particular model may bear little apparent relation to natural systems, theoretical progress in explaining the model may extend to progress in explaining other nonequilibrium systems. Models in which the equilibrium properties are thoroughly understood are often chosen. Then the specific effects of the forces driving the system out of equilibrium are readily apparent. General nonequilibrium systems present such complex time-dependence that physicists often prefer to study nonequilibrium steady state systems, those in which the distribution of states is independent of time. Even though much simplified, nonequilibrium steady state models still possess many counterintuitive properties. For example, a well understood equilibrium model is the Ising lattice gas [1]. A slight modification [2], introduced to drive it into nonequilibrium steady states, leads to remarkably different behavior.

The driven Ising model consists of a rectangular lattice with each site empty or occupied by a single particle. The dynamics is particle hopping to nearest neighbor empty sites. The rate of the hopping is controlled by the Ising Hamiltonian $\mathcal{H}$ and a bias in one direction, effectively a uniform DC “electric” field
$E$. Rates are chosen to satisfy a “local” detailed balance condition. That is, the net energy change due to a particle jump includes a local potential term, although a global electrostatic potential does not exist. To connect with the equilibrium system, these rates are consistent with the system being in contact with a thermal bath at temperature $T$ such that by setting $E = 0$, we recover the canonical $e^{-\beta E}/(\beta N)$ as the stationary distribution.

Many unexpected properties of the driven Ising model have been discovered, both for the original model and for its many variants [3]. Some of these behaviors have now been explained, but many are still not understood. For example, simulations show that the critical temperature $T_c(E)$ for the order-disorder transition increases with $E$ in the attractive driven Ising model [4]. This property is surprising, since one can easily argue as follows that the field will lower $T_c$. Because large fields would dominate over the interparticle attractions, they would effectively subject the system to additional noise. Thus a lower $T_c$ would be needed for the particles to cluster together and order. Further studies of the driven system have resulted in simple arguments in favor of an increased $T_c$ [5]. However, there is still no compelling reason to accept or reject the contradictory arguments. We lack an intuitive understanding that would enable us to make reliable predictions.

This project is a continuation of the study of similar systems [5, 6, 7] in an effort to find the underlying mechanisms giving rise to the mysterious phase diagrams. Specifically, we consider a driven Ising model with anisotropic interactions. That is, the interparticle interaction energies differ depending on whether the interaction is along or perpendicular to the field direction. This system has a complex phase diagram in the three dimensions of temperature, field, and anisotropy parameter.

The goals of this work are twofold. Firstly, we determine the phase diagram for the driven Ising lattice gas via Monte Carlo simulations. It is hoped that knowledge of the phase diagram will help increase basic understanding and intuition regarding nonequilibrium systems. Certainly the phase diagram provides a basis to which approximate theoretical solutions can be compared. Any truly successful theory or approximation must be able to predict phase diagrams such as this one. Also, the phase diagram may display unexpected phenomena that can lead to new questions of interest about nonequilibrium systems. Secondly, we explore the ability of high temperature series expansion techniques to locate the critical temperature.

1.2 Overview

A detailed description of the anisotropic driven Ising model follows in Chapter 2. Previously observed equilibrium characteristics are discussed. Chapter 3 deals
with Monte Carlo studies of the phase diagram. Details of how the Monte Carlo method is applied to this system are presented. We treat separately the cases of infinite (saturating) drive and finite drive. The main feature of the infinite drive system is a second order transition between ordered and disordered states. We locate the critical temperature via the standard method of observing the large fluctuations in structure factors that occur near criticality. However, certain data suggest the possible existence of an additional phase in the vicinity of this transition. A new order parameter is defined in an effort to detect this possible phase, and we discuss the results. When a finite drive is applied, the second order transition remains and a first order transition between two ordered phases also appears. Critical temperatures are determined using standard methods, as is the location of the first order transition line at higher temperatures. A novel method for locating the first order transition at lower temperatures is presented and its accuracy considered. In Chapter 4, we attempt to predict critical temperatures through a high temperature expansion. Details of the expansion are presented, and the results are compared and contrasted with the phase diagram found by Monte Carlo methods. Chapter 5 summarizes the results of the previous chapters and contains some discussion about the future of this work.
Chapter 2

The Model

2.1 Microscopic Description of the Model

The system studied consists of an \( L_x \times L_y \) square lattice. (See Figure 1 for a diagram.) Periodic boundary conditions are applied, so the model is in effect a torus. Sites on the lattice are labeled by \( \mathbf{r} = (x,y) \), where \( x \) and \( y \) are integers modulo \( L_x \) and \( L_y \), respectively. Each site is occupied by either an up spin or a down spin. Thus a configuration of the system can be specified by the set of spin numbers \( \{ s(\mathbf{r}) \} \), where \( s(\mathbf{r}) \) is +1 for an up spin and −1 for a down spin at site \( \mathbf{r} \). This model is equivalent to a particle/hole model via the relation \( n = \frac{1}{2}(s + 1) \), where \( n \) is the occupation number. The conversion maps up spins to particles \( (n = 1) \) and down spins to holes \( (n = 0) \). The terminology of the particle/hole model and the spin model will be used interchangeably in this thesis. However, all simulations were done for the spin model. While this choice does not change the phase diagram, it will affect magnitudes of structure factors and other such data. An important feature of our model is a conservation law: the number of particles is constant. In the spin system, this translates into \( \sum_{\mathbf{r}} s(\mathbf{r}) \) being fixed. To be able to access the critical point of the Ising model, we choose \( \sum s = 0 \). (This corresponds to half-filled systems, those in which \( \sum n = L_x L_y / 2 \).)

The system is given anisotropic nearest neighbor attraction between like spins and repulsion between opposite spins. Since the \( x \) direction will eventually be parallel to the field direction and the \( y \) direction transverse, let \(-J_\parallel\) be the interaction energy between like spins interacting in the \( x \) direction and \(-J_\perp\) the interaction energy between like spins in the \( y \) direction (with \( J_\parallel, J_\perp > 0 \)). Then the Hamiltonian is

\[
\mathcal{H} \equiv -J_\parallel \sum_{x,y} s(x,y) s(x+1,y) - J_\perp \sum_{x,y} s(x,y) s(x,y+1).
\] (2.1)
Anisotropy is introduced through the dimensionless anisotropy parameter $\alpha$:

$$J_{\parallel} = \alpha J \quad \text{and} \quad J_{\perp} = J/\alpha$$  \hspace{1cm} (2.2)

with $J$ representing the overall strength of the interactions. A field $E$ is applied in the negative $x$ direction. In the language of the particle-hole model, $E$ suppresses particle jumps antiparallel to the field direction and increases the probability of particle jumps along the field. Probabilities for transverse jumps are unaffected. Throughout this thesis, values for $E$ and for energies will be given in units of $J$.

![Diagram of the anisotropic driven Ising model and coordinate conventions used in this text.](image)

A typical equilibrium probability that two spins will exchange places is that of Metropolis [8]: \( \min\{1, e^{-\Delta \mathcal{H}/(k_B T)}\} \), where $\Delta \mathcal{H}$ is the change in energy due to the exchange, $T$ is temperature, and $k_B$ is Boltzmann’s constant. This exchange probability generalizes to the driven case as follows [2, 3]:

$$P = \begin{cases} 
\min\{1, e^{-\Delta \mathcal{H}/(k_B T)}\} & \text{for particle jumps transverse to } E \\
\min\{1, e^{-(\Delta \mathcal{H}+E)/(k_B T)}\} & \text{for particle jumps against } E \\
\min\{1, e^{-(\Delta \mathcal{H}-E)/(k_B T)}\} & \text{for particle jumps along } E.
\end{cases}$$  \hspace{1cm} (2.3)
2.2 Equilibrium Characteristics

Equilibrium characteristics of the Ising model are well understood in the thermodynamic limit [9, 10, 11]. Most prominently, the system undergoes a second order transition, from a disordered homogeneous phase (denoted by D) to a phase segregated state, when $T$ is lowered through the Onsager temperature $T_c(\alpha)$. (See Figure 2 for typical configurations of each phase and Figure 3 for the equilibrium phase diagram.) Expressed in units of $J/k_B$, $T_c(\alpha)$ can be obtained from the equation [12]

$$
(1 + \varepsilon^n) \left(1 + \varepsilon^{1/n}\right) = 2
$$

for $\varepsilon \equiv \exp\left[-2J/(k_BT_c(\alpha))\right]$. Specifically, $T_c(1) \approx 2.269 J/k_B$. Temperatures in this thesis will be given in units of $2.269 J/k_B$ so that $T_c(1) = 1$.

![Diagram of Ising model phases](image)

Figure 2. Examples of each of the three phases in the 30x30 equilibrium anisotropic Ising model: a) horizontal at $\alpha = 0.5, T = 0.7$; b) vertical at $\alpha = 3, T = 0.9$; c) disordered at $\alpha = 3, T = 2.0$. (Up spins are symbolized by ‘+’. For clarity, down spins are not displayed.)

Because the total spin is conserved, the ordered state at $T = 0$ will be a strip of like spins spanning the system. This strip will parallel either the $x$- or the $y$-axis to minimize the number of higher energy interactions (broken bonds) between unlike spins. States aligned with the $x$-axis (vertical strips) will be denoted by V, and states aligned with the $y$-axis (horizontal strips) will be denoted by H. The equilibrium ordered state is the one with the lowest interfacial free energy. This state is determined by the anisotropy parameter $\alpha$ and by the aspect ratio of the system, $L_y/L_x$. For $L_y/L_x = 1$, $\alpha = 1$ marks the phase boundary between the two states. The H-V boundary is associated
with a first order transition [13]. For general $L_y/L_x$, this boundary is located at that $\alpha(T)$ which satisfies $\sigma_x(\alpha,T)/\sigma_y(\alpha,T) = L_y/L_x$, where $\sigma_x$ is the surface tension (energy per unit length) for the vertical interface and $\sigma_y$ is the surface tension for the horizontal interface.

**Equilibrium phase diagram**

![Equilibrium phase diagram](image)

Figure 3. Phase diagram for the equilibrium anisotropic Ising model. The solid line indicates the critical temperature, and the dashed line indicates the first order transition.
Chapter 3

Monte Carlo Studies

3.1 The Monte Carlo Method

Monte Carlo simulations are used to determine the phase diagram for the anisotropic driven Ising model. The system starts in one of several standard configurations with zero magnetization. In each Monte Carlo step (MCS), $2L_xL_y$ bonds between nearest neighbor spins are chosen randomly (via a long period pseudorandom number generator). If the bond consists of two unlike spins, the pair is exchanged with probability \( \min \{1, \exp[-(\Delta H + E\delta x)/(k_B T)]\} \), where $\delta x$ is the change in $x$-coordinate (modulo $L_x$) of the up spin. (Cf. Equation 2.3.) Thus when the up spin attempts to move upward, against the field, $\delta x = +1$ and the exchange probability is reduced. Likewise, when the up spin attempts to move along the field, the exchange probability is increased. $\Delta H$ is computed from the number of bonds with nearest neighbor spins of the pair under consideration that will be broken or formed by the exchange of the spins. A random number between 0 and 1 is generated. If this number is less than the probability of the exchange, then the two spins are switched.

In a typical run, data from the first several thousand MCS is discarded while the system approaches steady state. (This number of MCS depends on the system size and is determined beforehand by observing time traces of measured values.) Then data is collected every 200 MCS until there are enough data points for computation of accurate averages.
3.2 System with Infinite Drive

We first consider what is perhaps the simplest case of the driven system, that in which the drive is infinite. When a random bond between an up spin and a down spin is chosen in the field direction, the up spin will always move downward, never upward. In practice, $E$ needs to be only large enough for saturation (i.e., the probability for an up spin to move downward is essentially 1 and the probability for an up spin to move upward is essentially 0). For the values of $\alpha$ used in these studies, $E = 50$ works quite well, overwhelming contributions of particle interactions to the effective energy changes. Horizontal strips should not survive, so the only ordered phase should be $V$. Thus the only feature of the $E = \infty$ phase diagram should be a second order transition between the $V$ and $D$ phases. The critical temperature for this transition should depend on the anisotropy parameter $\alpha$. We denote this temperature by $T_c(\alpha, E = \infty)$.

3.2.1 Locating second order transitions via peaks in fluctuations

Method

$T_c(\alpha, \infty)$ is located by standard methods. Every 200 MCS, we measure the Fourier transform of the spin $s(x)$,

$$\tilde{s}(k, p) \equiv \frac{1}{\sqrt{L_x L_y}} \sum_{x,y} s(x,y) \exp \left[ 2\pi i \left( \frac{kx}{L_x} + \frac{py}{L_y} \right) \right]$$

(3.1)

where $k, p$ are integers. Averaging over the rest of the run yields the structure factors,

$$S(k, p) \equiv \langle |\tilde{s}(k, p)|^2 \rangle.$$  \hspace{1cm} (3.2)

The structure factors are measures of how ordered the system is in a direction and with a frequency determined by $(k, p)$. In the disordered phase, they are of order 1. Below the critical temperature, the structure factors can be used to determine whether the system is in the H or V phase. When the system has H ordering, $S(1,0)$ is order $L_x L_y$ in the thermodynamic limit and $S(0,1)$ is small. When the system has V ordering, $S(0,1)$ is order $L_x L_y$ in the thermodynamic limit and $S(1,0)$ is small. In particular, for a perfectly formed vertical strip, $S(0,1) = (8L_x / L_y) / [1 - \cos(2\pi / L_y)]$ and $S(1,0) = 0$. For the H phase, the situation is reversed. Thus $S(0,1)$ and $S(1,0)$ may be used as order parameters.

The change of $S(0,1)$ from $O(L_x L_y)$ to $O(1)$ as $T$ increases certainly indicates that the order to disorder transition has occurred. However, since
this transition is continuous, \( T_c(\alpha, \infty) \) cannot be located precisely by simply observing changes in \( S(0,1) \). Therefore, we also measure the variance, 
\[ (\Delta S)^2 \equiv \langle |\hat{s}|^4 \rangle - S^2, \]
which plays a role similar to that of the magnetic susceptibility in equilibrium systems. For the \( S \)'s that are \( O(1) \), the associated \( \Delta S \)'s are expected to be just \( S \) itself [14]. Deep within the ordered phase, though some \( S \)'s will be \( O(L_x L_y) \), the \( \Delta S \)'s are expected to be still \( O(1) \). However, near a second order transition, the \( \Delta S \)'s diverge in the thermodynamic limit for the equilibrium system. This behavior of the \( \Delta S \)'s results from large scale fluctuations in the order parameter near the critical temperature. Similar fluctuations occur in finite systems, including driven systems. Fluctuations in finite systems cause an increase in the \( \Delta S \)'s to some larger value, though they do not actually diverge.

The above considerations lead to the following procedure for locating \( T_c(\alpha, \infty) \). We fix \( \alpha, E \) and perform separate simulations at several temperatures. At each \( T \), the simulation is started with some initial configuration and run for long enough that the system reaches a steady state. Then the run is continued for another 300K MCS while \( \hat{s}(k, p) \) data is collected every 200 MCS. (Specifically, running sums of \( |\hat{s}(k, p)|^2 \) are kept for \( k, p \) ranging from 0 to 5 and of \( |\hat{s}(k, p)|^4 \) for \( (k, p) = (0, 1) \) and \( (k, p) = (1, 0) \). This allows the calculation of \( S(k, p) \) for \( k, p \) ranging from 0 to 5, as well as \( [\Delta S(0, 1)]^2 \) and \( [\Delta S(1, 0)]^2 \). Trends in the various \( S(k, p) \) can be observed from this data.) After the run is complete, structure factors and variances are computed. Fluctuations in the structure factors occur near the critical temperature and cause the variance \( [\Delta S(0, 1)]^2 \) to become larger. A plot of \( [\Delta S(0, 1)]^2 \) versus \( T \) has a peak at some temperature that is identified as \( T_c(\alpha, \infty) \).

Results and discussion

We initially restrict our studies to a 30×30 lattice so that simulations can be run in a reasonable time period. Starting with random configurations, we perform 400K MCS runs for \( \alpha = \frac{1}{2}, \frac{1}{3}, \frac{2}{3}, 1, \frac{4}{3}, 2, 3 \) and \( 0.5 \leq T \leq 3.0 \). (It is felt that setting \( \alpha < \frac{1}{5} \) or \( \alpha > 3 \) will not produce useful results in systems of this size.) Spacing of temperatures for these runs varies but is brought as low as 0.025 near the peak in \( [\Delta S(0, 1)]^2 \) to allow precision in determining the critical temperature. Runs last a total of 400K MCS, with data from the first 100K MCS discarded to allow the system to reach steady state.

As anticipated, we find that \( S(0,1) \) grows substantially when \( T \) is lowered (Figure 4), as do the other \( S(0, p) \) (\( p \) odd). The remaining structure factors remain approximately constant. \( [\Delta S(0, 1)]^2 \) does indeed peak at a temperature for which the system is transitioning from large to small \( S(0, 1) \) (Figure 5). (See Figure 6 for typical configurations of ordered and disordered nonequilibrium states.) Identifying the transition temperature through the peak in \( [\Delta S(0, 1)]^2 \), we find the second order transition line \( T_c(\alpha, \infty) \) to be a monotonically decreasing...
ing function of $\alpha$, as shown in Figure 7. (The theoretical result for $T_c(\alpha, 0)$ for an infinite system is also shown for purposes of comparison. However, note that the equilibrium system may order into either the H or V phase, depending on whether $\alpha < 1$ or $\alpha > 1$, while the infinitely driven system can order only into V. Finite size effects are discussed in more detail below, but the curve for a finite system should be similar.) This monotonically decreasing behavior contradicts previous conjectures [5], showing that our intuitive picture, based on the competition of long and short ranged correlations, is still unreliable. Also surprisingly, the critical temperature is not always greater than that for the equilibrium system.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure4}
\caption{$S(0,1)$ versus $T$ for a $30 \times 30$ system at $\alpha = 2$ with infinite drive. The decrease in $S(0,1)$ as $T$ increases is indicative of a second order transition.}
\end{figure}
Figure 5. $[\Delta S(0,1)]^2$ versus $T$ for a 30 x 30 system at $\alpha = 2$ with infinite drive. The peak in the variance of $S(0,1)$ indicates that the critical temperature is $T_c(2, \infty) = 0.975$.

Figure 6. Representative configurations for a 30 x 30 $\alpha = 2$ system with infinite drive: a) well below $T_c$ at $T = 0.7$; b) at criticality at $T = 0.975$; c) well above $T_c$ at $T = 1.4$. 

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Figure 7. Phase diagram for the $30 \times 30$ anisotropic Ising model with infinite drive. The equilibrium critical temperature line (theoretical result for infinite system size) is shown for reference.

The uncertainties associated with this $T_c(\alpha, \infty)$ are actually much larger than the minimum temperature step size of 0.025. For $T$ greater than the approximate $T_c(\alpha, \infty)$, $S(0, 1)$ does not decrease in a simple way, especially for systems with large $\alpha$. In these cases, as $T$ is increased, we often observe breakup of a single strip into two-strip or multi-strip states. As a result, when $T$ is increased through this $T_c(\alpha, \infty)$, not only does $[\Delta S(0, 1)]^2$ become large; $S(0, 2)$ sometimes increases by as much as an order of magnitude. Typically, at temperatures $\sim$30% higher than $T_c(\alpha, \infty)$, we can be quite certain that the system is disordered. However, at intermediate temperatures the system may have a fair amount of long range order in the field direction. This observation leads to the question of whether another phase that is ordered in the field direction and disordered in the transverse direction might exist between V and D. To consider this possibility, we later define and discuss in detail a new order parameter.

The above phase diagram was found using $30 \times 30$ systems only. However, true phase transitions accompanied by thermodynamic singularities are properties of infinite systems. Any conclusions regarding the thermodynamic limit would rely on either simple extrapolations or finite size scaling. Limited computational power prevented extensive study of the effects of finite size, but we
obtained some results by studying 60×60 and 90×90 systems at the extreme α’s (α = 1, 2, 3). Critical temperatures for these systems were again determined by the peak in [ΔS(0, 1)]², so they are sensitive only to the breakup of the single strip state. “Completely disordered” states occur at somewhat higher temperatures.

The larger systems require longer time periods to reach steady state. Observations of time traces of “instantaneous structure factors,” [\tilde{s}(k, p)]² (cf. Equation 3.1), indicated that the following length runs allowed the system to stabilize before data was collected. 60×60 systems were started with random configurations, and the first 400K MCS were discarded. The simulation lasted 700K MCS so that the usual 300K MCS of data could be collected. Spacing between temperature points near the critical temperature was 0.5. This method had to be modified somewhat for 90×90 systems, which took extremely long times to order. 90×90 system runs were started at temperatures about 0.5 below the 30×30 \( T_c(\alpha, \infty) \) with either a single vertical strip or a random configuration. (The initial configuration depended on whether or not the random configuration could reach steady state as quickly as desired. If not, the vertical configuration was used.) Simulations were run until time traces of “instantaneous structure factors” indicated that a steady state had definitely been reached at that temperature (about 400K to 500K MCS). The final configuration was used as the initial configuration of the next run, which had a temperature 0.5 higher. This next run lasted a total of 500K MCS, with the first 200K MCS discarded and data taken for the remaining 300K MCS. Its final configuration became the initial configuration for the next 500K MCS run with the temperature raised another 0.5 units. This process of using the final configuration of one run for the initial configuration of the next run at a higher temperature continued until [ΔS(0, 1)]² peaked and then declined.

\( T_c(\alpha, \infty) \) results for the various system sizes are shown in Table 3.1. Similar to the equilibrium cases, these transition temperatures tend to increase with larger system sizes. The critical temperatures appear to be asymptotically approaching values that are somewhat above the \( T_c(\alpha, \infty) \) for 30×30 systems, but the monotonically decreasing trend of the \( T_c(\alpha, \infty) \) line remains. Based on these studies, we believe that the general features of the phase diagram (Figure 7) will survive in the thermodynamic limit.

<table>
<thead>
<tr>
<th>( L )</th>
<th>( \alpha )</th>
<th>1/3</th>
<th>1/2</th>
<th>2</th>
<th>3</th>
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<td>1.05</td>
<td>0.80</td>
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</tbody>
</table>

Table 3.1: \( T_c(\alpha, \infty) \) for systems with various \( L = L_x = L_y \).
3.2.2 Examining transition region via new order parameter $R$

Some of our simulations display unusual phenomena suggestive of the possible existence of another phase in which the system is ordered in one direction but not in the other. We discuss these observations and define a new order parameter which would be sensitive to the existence of such a phase.

Motivation

In some simulations at large $\alpha$ values, especially for large system sizes, the system appears to be somewhat ordered in the field direction but not in the transverse direction. In essence, it appears “stringy.” Figure 8 shows a typical configuration.

The two-point correlation function between spins separated by a displacement $\mathbf{r}$ is $G(\mathbf{r}) = \langle \sigma_0 \sigma_r \rangle$. In equilibrium systems, the correlation functions are known exactly. For $\alpha > 1$, the correlations are greater in the vertical direction than in the horizontal direction. The effect of the drive is to increase correlations in the field (vertical) direction and to decrease correlations in the transverse (horizontal) direction. The correlation lengths decrease with increasing temperature, an example of which is shown in Figure 9. It is conceivable that in the driven system at some temperature, the correlations in the vertical direction might be sufficiently strong to induce ordering into vertical clusters (“strings”) but that the correlations in the transverse direction might be too weak to bring the strings together into a single ordered strip.

To look more closely at this idea, we consider frequency histograms of the column density, the number of up spins in a column. The number of times each column density occurs is recorded over all the data points (every 200 MCS) of a run and over all the columns in the system, and a frequency histogram is generated from this information. The column density histogram for a vertically ordered 30×30 system has peaks near 0 and 30 up spins, since most of the columns are of uniform spin type. At high temperatures, the column density histogram is a Gaussian centered at 15 spins, half filling. Figure 10 shows column density histograms at several temperatures. For that system, $T_c(3, \infty) = 0.75$. Below $T_c$, evidence of ordering in the vertical direction is clearly visible from the histograms. Even as high as $T = 0.9$, the column density histogram is still bimodal, rather than Gaussian, indicating that some ordering in the vertical direction survives. However, the structure factors indicate that very little of the single strip state remains. These observations support the idea that systems may order into a stringy state.
Figure 8. A typical “stringy” configuration, appearing ordered in the field direction but not the transverse direction, in a $90 \times 90$ system at $\alpha = 3, T = 0.85, E = 50$. 
Figure 9. A plot of the correlations $G$ as a function of distance in the $x$-direction at $\alpha = 3$ and several temperatures. $G$ decreases as the temperature is raised.

**Definition of $R$**

To quantify these ideas, we define a new order parameter based the ratio of the correlation function $G(L/2, 0)$ to the structure factor $S(0, 1)$:

$$ R \equiv L^d \frac{G(L/2, 0)}{S(0, 1)} \quad (3.3) $$

where $L (= L_x = L_y)$ is the length of the sides and $d$ is the dimension of the system (2 in these studies). Roughly, we expect $R$ to be sensitive to stringy states in which there are long range correlations in the field direction but $S(0, 1)$ is small because there is not single-strip ordering.

A detailed analysis confirms that $R$ should display distinct behavior in a stringy phase, were one to exist. Far into the disordered phase, the correlation function decays as a power law: $G(L/2, 0) \sim O(L^{-d})$ [18]. Under these conditions, $S(0, 1) \sim O(1)$. Then at high temperatures, we expect

$$ R \sim O(1). $$

Next page: Figure 10. Column density frequency histograms for a $30 \times 30$ system at $\alpha = 3, E = 30$ and several temperatures (0.5, 0.7, 0.9, and 2.0). $T_c$ is 0.75 here. The data was taken every 200 MCS over the last 300K MCS of a 400K MCS run.
Near criticality, if there are no stringy states, we may use the results of
renormalization group analysis [15], which says that
\( G(0, r) \sim r^{-\frac{(d-2+\Delta)}{1+\Delta}} \)
and \( S(0, p) \sim p^{-2} \). Then \( R \sim O(L^{\frac{(d-3)\Delta}{1+\Delta}}) \). \( \Delta \), the anisotropic exponent,
is \( (8 - d)/3 \) here, so in \( d = 2 \) we expect
\[
R \sim O(L^{-2/3})
\]
close to the critical temperature. Far into the ordered phase, \( G(L/2, 0) \sim O(M^2) \) and \( S(0, 1) \sim O \left[ (M/\pi)^2 L^d \right] \), where \( M \) is the magnetization. Then at
low temperatures, we expect
\[
R \sim O(1).
\]

On the other hand, in a stringy state, ordering in the vertical direction would
cause \( G(L/2, 0) \sim O(1) \). The system would not have formed a single strip state,
so \( S(0, 1) \sim O(1) \). Then if the system were in a stringy state, we would see
\[
R \sim O(L^d).
\]

Only a stringy state would cause \( R \) to increase with \( L \). Our approach, then,
is to run simulations for varying system sizes in which both \( G(L/2, 0) \) and \( S(0, 1) \) data is collected. We use the averages of \( G(L/2, 0) \) and \( S(0, 1) \) to compute
\( R \), rather than computing instantaneous \( R \) values and averaging at the end,
because the instantaneous \( R \) can be disproportionately inflated by occasional
fluctuations in which the system becomes highly disordered and \( S(0, 1) \) drops
to a very small value.

Results and discussion

We followed the above procedure to search for stringy states at \( \alpha = 3, E = \infty \). System sizes used were \( 10 \times 10, 20 \times 20, 30 \times 30, 40 \times 40, 60 \times 60 \), and
\( 90 \times 90 \). Temperatures studied were \( T = 0.7, 0.75, 0.8, 0.85, 0.9, 2.0 \). The critical
temperature found from the peak in the variance of \( S(0, 1) \) was 0.75, so this
range included the critical temperature and temperatures slightly above it where
stringy states might occur. The smaller systems were started with random
configurations. The \( 60 \times 60 \) runs were started \( V \) so that they would not become
stuck in a metastable multi-strip state at low temperatures. The \( 90 \times 90 \) runs
were started \( V \) at the lowest temperature, and then their final states were used as
the initial configuration for the next higher temperature and so on. This helped
minimize the number of MCS required for the large system to reach steady state.
Simulations ranged in length from 400K to 800K MCS. In all cases, observations of
“instantaneous structure factor” time traces indicated that those run times
would be long enough for the system to reach steady state. Except for \( T = 2.0 \),
at least 3 independent runs were done at each temperature and for each system
size. (The \( T = 2.0 \) data was taken to only verify that our prediction for \( R \) values
at high temperatures was approximately correct. Therefore, 1 or 2 independent runs were deemed sufficient for points on the $T = 2$ curve.)

Figure 11 displays the results for $\mathcal{R}$ versus $L^2$. At two of the temperatures studied, $T = 0.85, 0.9$, $\mathcal{R}$ appears to increase with $L$. Specifically, $\mathcal{R}$ appears to be order $L^2$, especially at $T = 0.85$, where least squares analysis of $\mathcal{R}$ versus $L^2$ yields a correlation coefficient of 0.996. At temperatures other than $T = 0.85, 0.9$, $\mathcal{R}$ appears to be approximately order 1. (It should be noted that the data point for $T = 0.7$, $10 \times 10$ systems, $\mathcal{R} \approx 17$, has been omitted from Figure 11 for greater clarity. The $\mathcal{R}$ value there is high because of unexpectedly metastable two-strip states. We suspect the very small system size may have contributed to this unusual data point but do not yet have a good explanation for its occurrence.)

![Graph](image)

Figure 11. Plot of $\mathcal{R} = \frac{C(L/2,0)}{S(0,1)}$ versus $L^2$ at various temperatures.

Figure 11 seems fairly consistent with the existence of stringy states. However, for a true stringy phase to exist, the $\mathcal{R} \sim O(L^\alpha)$ behavior must persist in the thermodynamic limit of infinite system size. That this will occur is by no means guaranteed. Even an equilibrium system can appear stringy under appropriate conditions. For example, the equilibrium $30 \times 30$ system with $\alpha = 3, T = 1.35$ (slightly above criticality) shown in Figure 12 appears visibly stringy. This fact is understandable when one realizes that the correlation length in the $x$-direction, 15.1, is long enough to span the system but that the correlation length in the $y$-direction, 3.8, is not long enough to span a single vertical strip state. Due to the equilibrium correlation function’s exponential
decay with distance, we would not expect to see stringy behavior in a 60 \times 60
system under the same conditions. Certainly the equilibrium Ising model does
not have a stringy phase in the thermodynamic limit. However, driven systems
have displayed many surprising phenomena that are not found in equilibrium
systems. We conjecture that stringy states will survive even in larger systems
and persist as a separate phase in the thermodynamic limit.

Constraints on computing power prohibited the study of systems larger
than 90 \times 90. Further research in this area should involve a continuation into
very large system sizes to determine whether the \( R \sim O(L^d) \) dependence still
holds. Additionally, frequency histograms of \( S(0, 1) \) and \( S(0, 2) \) have displayed
some unusual features that might be attributed to the presence of multi-strip
("stringy") states. More detailed study should reveal whether or not this ex-
planation is reasonable.

![Figure 12. 30 \times 30 equilibrium system configuration at \( \alpha = 3, T = 1.35 \) that appears relatively ordered in the field direction and relatively disordered in the transverse direction.]

3.3 System with Finite Drive

As stated earlier, the equilibrium anisotropic Ising model has three phases, H,
V, and D. A first order transition occurs at low temperatures between two or-
dered phases, and as temperature is increased, a second order transition occurs
between the ordered phases and a disordered phase. We expect finite, nonsat-
urating drives to deform the equilibrium phase diagram continuously toward
the infinite drive phase diagram. This behavior does indeed transpire as \( E \) is
increased. We discuss below our methods and results for systems with finite
drive.
3.3.1 First order transitions

For $\alpha < 1$, horizontal strips can survive if $E$ is small enough that it cannot
overcome the large attractive forces between the spins in a horizontal strip.
Thus for small values of $E$, there is still a first order transition between H and
V phases. When $E = 0$, the transition line lies along the $\alpha = 1$ line. The
transition line should move toward the left (smaller $\alpha$) when $E$ is increased.
The $\alpha$ value for the first order transition will be denoted by $\alpha_1(T, E)$.

Hysteresis loop method for higher temperatures

When $T$ is not too low, the transition from vertical to horizontal ordering can
be located by looking at a characteristic property of first order transitions: hysteresis loops. The shifted transition line in the phase diagram should roughly
parallel the $T$ axis. Hence it is reasonable to search for this transition by sweeping $\alpha$ while $T$ and $E$ are held fixed. The system orders horizontally at small $\alpha$.
When $\alpha$ increases, horizontal ordering remains as a metastable state, but eventu-
ally the metastable state decays and the system switches to vertical ordering
when $\alpha$ becomes sufficiently large. Likewise, the system orders vertically for
large $\alpha$, but it eventually switches to horizontal ordering when $\alpha$ becomes small
enough.

As a measure of how the system is ordered, we monitor the ratio

$$r = \frac{S(0,1) - S(1,0)}{S(0,1) + S(1,0)}, \quad (3.4)$$

which can range between $+1$ (perfect vertical ordering) and $-1$ (perfect hori-
izontal ordering). A 30×30 system is started with horizontal ordering and $\alpha$
increased in steps of 0.025. After each increase, the system is evolved for 200K
MCS. When $\alpha$ becomes sufficiently large, $r$ suddenly jumps from a negative
number near -1 to a positive number near +1 as the metastable horizontal strip
decays (Figure 13). The $\alpha$ value for this switch should certainly be above
$\alpha_1(T, E)$. Similarly, the system is started with vertical ordering, and $\alpha$ is de-
creased in steps of 0.025 and the system evolved for 200K MCS at each step.
When $\alpha$ becomes sufficiently small, $r$ suddenly jumps from a positive number
near +1 to a negative number near -1. This $\alpha$ should be below $\alpha_1(T, E)$. We
estimate $\alpha_1(T, E)$ by averaging the values of $\alpha$ where the jump occurs.

This method works well at temperatures not too far below $T_c(\alpha, E)$. It was
used to find $\alpha_1(T, E)$ for $E = 1, T = 0.9, 0.8$ and $E = 2, T = 1.0, 0.9$, since
the method produces hysteresis loops no wider than about 0.125$\alpha$ under those
conditions. Results for $\alpha_1(T, E)$ are contained in the full phase diagram for
finite $E$, Figure 15. However, for lower $T$, the lifetimes of metastable states are
too long and hysteresis loops become too wide to be reliable. For example, at
$E=2, T=0.8$, the hysteresis loop spans $0.3\alpha$, corresponding to 36% of the total $\ln\alpha$ range studied ($\alpha = 1/3$ to $\alpha = 3$). Such loops will likely not yield accurate estimates of the $\alpha$ value for the first order transition. For this reason, another method is needed to determine the location of the first order transition at lower temperatures.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{hysteresis_loop.png}
\caption{Hysteresis loop formed by a $30 \times 30$ system at $T = 0.8, E = 1$ when $\alpha$ is increased in steps of 0.025 from a horizontal state ($r \sim -1$) and decreased in steps of 0.025 from a vertical state ($r \sim +1$).}
\end{figure}

**Saddle point method for lower temperatures**

For equilibrium systems, the notion of free energy landscapes, though not mathematically rigorous, can be very helpful in building intuitive pictures for what may occur dynamically. In particular, they are often used for discussing metastable states and first order transitions. A specific example is the Ising model (with no conservation constraint) far below criticality, undergoing a first order transition when an external *magnetic* field reverses sign. Here, the stable state is just the one with magnetization aligned with the field, while the metastable one has the opposite magnetization. In the vicinity of the transition, both states are associated with deep “wells” in the free energy landscape. Between the two wells should be at least one saddle point (mountain pass). Even though the metastable well is somewhat shallower than the stable one, a system can spend exceedingly long times in the former before a sufficiently large (thermal) fluctuation takes it over the pass and into the stable well. Since the saddle point
“connects” the two wells, its associated configuration must share the characteristics of both the stable and the metastable phase. For the Ising model, this turns out to be a droplet of the stable phase in a “sea” of the metastable phase [16]. Clearly the height and width of the saddle point will dictate the probability for such a transition and therefore the lifetime of the metastable state. Using these notions, it is possible to estimate these life times for the Ising model, given a specific microscopic dynamics.

Though our driven lattice gas is a nonequilibrium system, we believe that the notion of landscapes is still useful. Thus, we imagine that near $\alpha_1$ at low $T$, deep wells are associated with both horizontal and vertical strip states. To make the transition from one to the other, the system may find itself having to pass a saddle point configuration. Based on the arguments above, we propose two configurations, which “connect” the vertically and horizontally ordered states, as possible candidates for the saddle point. Figure 14a shows the most symmetric configuration. Though less symmetric, the configuration shown in Figure 14b has less interface between the phases. In fact, the latter can be viewed as a droplet of one phase (white) embedded in a “sea” of the other.

For very low temperatures, it would take prohibitively long runs to determine which state is more stable (or which well is “deeper” in the language of landscapes). However, we can explore the landscape around the saddle point more easily. The hope is that the topography of the landscape around this point reflects to some extent which well is deeper. To be precise, we conjecture that a system which starts at the saddle point will evolve to the deeper well with higher probability. The transition line $\alpha_1(T, E)$ is then determined as that set of parameters $(\alpha, T, E)$ for which a saddle point configuration evolves, with equal probability, into both the vertical- and horizontal-strip states. Let us emphasize that, although this method is not guaranteed to identify the location of the first order transition, it should be a reasonably good indicator.

Applying this method to determine $\alpha_1(T, E)$ requires a means of deciding whether a configuration is ordered horizontally or vertically. We chose to do this by comparing the “instantaneous structure factors” $\langle s(0,1) \rangle^2$, $\langle s(1,0) \rangle^2$, $\langle s(0,2) \rangle^2$, and $\langle s(2,0) \rangle^2$ to their average steady state values for ordered configurations under the same set of conditions. The criterion that the conditions be the same is an important one, since average steady state values of structure factors depend on $(\alpha, T, E)$. For example, a system at $T = 0$ will order into perfect strip, but at higher temperatures, systems will be imperfectly ordered. Thus we need accurate values of the averages and standard deviations of the structure factors (in the steady state) first. To determine these, we carry out 400K MCS runs for each parameter set $(\alpha, T, E)$ in a region around the initial guess for $\alpha_1(T, E)$. In these runs, the system were started in an ordered configuration (one strip, vertical or horizontal) and remained in the same stable (or metastable) state for the duration of the run. Runs in which the system underwent large fluctuations from the appropriate ordered state were discarded.
Standard deviations of the structure factors were also collected. For the standard deviation in \( S(0, 1) \) or \( S(1, 0) \), whichever is large for the ordered state under consideration, the methods of Section 3.2.1 were used. The standard deviation in the other structure factors equals the structure factor itself [14].

With good characterization of the stable and metastable states, we proceeded to study systems starting at the saddle point. First, we used an “X” shape (or Saint Andrew’s cross, Figure 14a) as a putative configuration near the saddle point. To see if substantial differences in the estimated \( \alpha_1(T, E) \) would result from choosing other configurations as the saddle point, we used another highly symmetric intermediate configuration: an “L” (Figure 14b). Both configurations possess a high degree of order and appear intermediate between the \( H \) and \( V \) states. The program implementing the “X” and “L” configurations was designed carefully to maximize symmetry in the discrete \( L_x \times L_y \) system and to avoid biasing the result towards either \( H \) or \( V \). In these studies, \( 30 \times 30 \) lattices were used with both initial configurations (“X” and “L”). As will be reported in detail below, no major differences in \( \alpha_1 \) are found.

![Figure 14: (a) “X” and (b) “L” configurations, possible saddle points between vertical and horizontal ordering.](image)

To compare this new method to the standard hysteresis loop method, we chose to study \( E = 1, T = 0.8 \). To see how the first order transition line found from hysteresis loops extends downward at lower temperatures, we chose three additional values of \( T \) to study: 0.65, 0.70, and 0.75. For \( E = 1 \), we focused on the values \( \alpha = 0.65, 0.70, 0.75 \), and 0.80. For \( E = 2 \), we used \( \alpha = 0.40 \),
Table 3.2: Number of runs (out of 200) that were started in “X” configuration
and ordered vertically for \( E = 1 \) and various values of \( \alpha, T \).

<table>
<thead>
<tr>
<th>( T ) ( \alpha )</th>
<th>0.65</th>
<th>0.70</th>
<th>0.75</th>
<th>0.80</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.65</td>
<td>27</td>
<td>75</td>
<td>182</td>
<td>198</td>
</tr>
<tr>
<td>0.70</td>
<td>14</td>
<td>74</td>
<td>165</td>
<td>197</td>
</tr>
<tr>
<td>0.75</td>
<td>15</td>
<td>77</td>
<td>154</td>
<td>200</td>
</tr>
<tr>
<td>0.8</td>
<td>16</td>
<td>77</td>
<td>148</td>
<td>200</td>
</tr>
</tbody>
</table>

Table 3.3: Number of runs (out of 200) that were started in “X” configuration
and ordered vertically for \( E = 2 \) and various values of \( \alpha, T \).

<table>
<thead>
<tr>
<th>( T ) ( \alpha )</th>
<th>0.40</th>
<th>0.45</th>
<th>0.50</th>
<th>0.55</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.65</td>
<td>36</td>
<td>101</td>
<td>148</td>
<td>189</td>
</tr>
<tr>
<td>0.70</td>
<td>69</td>
<td>142</td>
<td>176</td>
<td>196</td>
</tr>
<tr>
<td>0.75</td>
<td>89</td>
<td>172</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

0.45, 0.50, and 0.55. Starting with the “X” configuration, we carried out 200
independent runs under each set of conditions \( (\alpha, T, E) \). \( |\hat{s}(0, 1)|^2, |\hat{s}(1, 0)|^2, \)
\( |\hat{s}(0, 2)|^2, \) and \( |\hat{s}(2, 0)|^2 \) were measured every 200 MCS. Each run terminated
when 10 consecutive measurements (i.e., over a period of 2,000 MCS) of the
four “instantaneous structure factors” fall within 3 standard deviations of the
average \( S \)’s for either vertical or horizontal ordering. At that point, the system
was ordered with either a vertical or a horizontal strip. The fraction of runs
which terminated in the vertical state (as determined by \( S(0, 1) > S(1, 0) \))
was recorded. As expected, this fraction increases monotonically with \( \alpha \) (at
fixed \( T, E \)). The points where this fraction is 1/2 (as determined by linear
extrapolation) were considered part of the line of first order transitions between
horizontal and vertical ordering.

The “X” configuration is considered first. The number of runs (out of 200)
for which the system ordered vertically is shown in Tables 3.2 \( (E = 1) \) and 3.3
\( (E = 2) \). Linear extrapolation between the two \( \alpha \) values surrounding where
100 runs would order vertically is used to extract \( \alpha_1(T, E) \). The hysteresis loop
method found that \( \alpha_1(0.8, 1) = 0.70 \), and the saddle point method (with “X”
as the saddle point) gives \( \alpha_1(0.8, 1) = 0.72 \). These two values are in fairly
good agreement, differing by only 3%, which is also 20% of the width of the hysteresis
loop (see Figure 13). Thus it appears that the saddle point method produces
valid results for \( \alpha_1(T, E) \) when the “X” initial configuration is used.

The “L” starting configuration does not fare as well, however. Results from
the “L” starting configuration for \( E = 1 \) are displayed in Table 3.4. In this case,
the saddle point method gives \( \alpha_1(0.8, 1) = 0.75 \), as opposed to the 0.70 found
via the hysteresis loop method. This answer is clearly somewhat incorrect, since
the hysteresis loop of Figure 13 shows that a system started in an H state at

26
Table 3.4: Number of runs (out of 200) that were started in “L” configuration and ordered vertically for $E = 1$ and various values of $\alpha, T$.

<table>
<thead>
<tr>
<th>$T \setminus \alpha$</th>
<th>0.65</th>
<th>0.70</th>
<th>0.75</th>
<th>0.80</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.65</td>
<td>0</td>
<td>24</td>
<td>156</td>
<td>192</td>
</tr>
<tr>
<td>0.70</td>
<td>1</td>
<td>13</td>
<td>108</td>
<td>186</td>
</tr>
<tr>
<td>0.75</td>
<td>0</td>
<td>13</td>
<td>88</td>
<td>200</td>
</tr>
<tr>
<td>0.8</td>
<td>1</td>
<td>17</td>
<td>99</td>
<td>200</td>
</tr>
</tbody>
</table>

low $\alpha$'s changes to a V state when $\alpha$ is increased to 0.75. Relative to the “X” configuration, the “L” configuration favors ordering into H states, especially at higher temperatures.

From comparison of the $\alpha_1(0.8, 1)$ values obtained via the hysteresis loop method and the saddle point method, we conclude that the saddle point method can be useful in locating first order transition lines, as long as one chooses a saddle point configuration carefully. Configurations that appear to be equally good choices can produce somewhat different results, so comparison with higher temperature hysteresis loop results is important. In any case, all three calculations of $\alpha_1(0.8, 1)$ are within less than 10% of each other, which gives us some confidence in quoting $\alpha_1(T, E)$. Future studies to determine why the “L” configuration, more so than the “X”, favors ordering into H states may provide some insight into how one can best choose possible saddle point configurations.

Because of the greater accuracy of the results obtained with the “X” configuration, the “X” results for $\alpha_1(T, E)$ at lower temperatures are those displayed in the finite drive phase diagram (Figure 15).

### 3.3.2 Second order transitions

In our studies of the second order transition line for small drives, we again used 30x30 lattices. We located the transition line via the same method as for an infinite drive: running simulations at various temperatures and looking for peaks in the variance of structure factors. For small drives, however, the ordered phase can be either V or H, depending on which side of the $\alpha_1(T, E)$ line the $\alpha$ under consideration falls. Thus a peak in $[\Delta S(0, 1)]^2$ indicated the critical temperature for $\alpha > \alpha_1(T, E)$ and a peak in $[\Delta S(0, 1)]^2$ indicated the critical temperature for $\alpha < \alpha_1(T, E)$.

As with the infinite drive studies, simulations were run for 400K MCS with the first 100K MCS discarded so that the system could reach steady state. Data taking occurred every 200 MCS. Spacing between temperature points was brought as low as 0.025 near the critical temperature. The small drives studied were $E = 1, 2, 5$. The usual $\alpha = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1, \frac{5}{4}, 2, 3$ were used, and to gain a better
understanding of the phase diagram near the bicritical points, we also looked at \( \alpha = 0.57, 0.65 \) for \( E = 1, 2 \).

As shown in Figure 15, the behavior of \( T_\alpha(\alpha, E) \) is quite complex. For \( \alpha = 3 \), \( T_\alpha \) first increases and then decreases towards the low value of \( T_\alpha(3, \infty) \) found above. For \( \alpha = 1 \), the known monotonic increase of \( T_\alpha \) is confirmed [2]. In its neighborhood, both \( T_\alpha(\frac{3}{2}, E) \) and \( T_\alpha(\frac{4}{3}, E) \) appear to increase monotonically with \( E \) as well. In the \( \alpha = \frac{4}{3} \) case, the ordered phase becomes \( V \) as soon as the small field \( E = 1 \) is applied, despite the fact that \( \alpha < 1 \). This reflects the known effect of the drive: setting up positive long range correlations along the drive and thus favoring vertical strips. For \( \alpha < \frac{3}{2} \) and the values for \( E \) that we studied, the system orders into either \( V \) or \( H \) depending on the drive. For those cases where the ordered phase is \( H \), it is unexpected that \( T_\alpha(\alpha, E) \) is still greater than the equilibrium \( T_\theta(\alpha, 0) \). Since the drive is known to reduce correlations in the transverse direction, we must find a new argument for how ordering into \( H \) could occur at a higher temperature when the drive is applied. In light of the ideas presented above regarding stringy states, one might hypothesize that perhaps the correlations in the parallel direction are the key factor in determining when the system can order into horizontal strips. The correlation length in the transverse direction might be long enough to induce ordering into horizontal strings at equilibrium, but the drive is needed to increase correlations in the vertical direction so that the strings can come together into a single horizontal strip. This idea is easily checked by comparing row density histograms at, for example, \( E = 0 \) and \( E = 2 \) with \( T \) values near \( T_\theta(\frac{3}{2}, E) = 1.1 \). The row density histograms have distinct differences indicating that the drive does indeed induce ordering in the transverse direction, not just the parallel direction. So this explanation fails. Simulation results again highlight the lack of reliable intuition about driven systems.

The behavior of \( T_\alpha(\alpha, E) \) becomes particularly complicated near the bicritical point. \( T_\alpha(\alpha, E) \) dips in the vicinity of the bicritical point. As a result, for fixed \( \alpha \), it first increases with \( E \) (while ordering into \( H \)), then decreases to a minimum value \( T_B \) at the bicritical point, and finally increases again with stronger drives. To the level of accuracy of these studies, \( T_B \) is approximately the same as \( T_\theta(\alpha, 0) \), though we have no reason to believe that they should be equal.
Figure 15. Phase diagram for the $30 \times 30$ anisotropic Ising model with finite drives. The equilibrium critical temperature line (theoretical result for infinite system size) is shown for reference. Solid lines indicate critical temperatures, and broken lines indicate first order transitions.

**Additional comments for $E=5$**

For $E=5$, all of the ordered states we have observed are $V$, so we have never explored the line of first order transitions. It is possible that first order transitions occur just outside the range of $\alpha$'s we have used. Indeed, the slight dip of $T_c(\alpha,5)$ at $\alpha = \frac{1}{5}$ is actually due to quite complicated behavior. For $T \geq 1.6$, $S(1,0) > S(0,1)$, even though the system actually orders into $V$ for $T \leq 1.5$, i.e., $S(0,1) > S(1,0)$. In this region of temperatures, the fluctuations in both structure factors are quite large. For these reasons, the $T_c(\frac{1}{5},5)$ data point was found to a maximum precision of only 0.1, instead of the 0.025 of the other $T_c(\alpha,E)$ points. It is possible that $\alpha = \frac{1}{5}$, $T \approx 1.55$ is very close to the bicritical point. In fact, a first order transition line $\alpha_1(T,5)$ with slope similar to that of $\alpha_1(T,2)$ might account for the increase in $S(1,0)$ as $T$ is increased. To explore further the idea of a first order transition in this region, we would need to set $\alpha < \frac{1}{5}$. Obtaining accurate results in such a highly anisotropic system would require larger lattices, a task which lies outside our present computational capabilities.
Chapter 4

High Temperature Series Expansion Studies

Although the driven lattice gas model was introduced 15 years ago, there is still no reliable approach to predict the general features of the phase diagram. One method that has been used previously to estimate the critical temperature is the study of the steady state two-point correlation function $G(r)$ in a first order “high temperature” expansion [17], which is actually an expansion in small $J$ or $K = J/(k_BT)$. In this approach, an approximate equation for $G(r)$, first derived in [18], is solved exactly. The previous study, which dealt with only the isotropic case, suggested that this method might be effective in making qualitative predictions of the phase diagram. A first order expansion would certainly not be expected to attain quantitative accuracy. However, using the high temperature expansion technique for the isotropic driven Ising model reproduced the qualitative result that $T_c(E)$ increases monotonically with $E$. To assess further the efficacy of this method, we extend the calculations to the anisotropic case and compare the predicted $T_c(\alpha, E)$ with that found in simulations. The first section of this chapter outlines the high temperature expansion method. Details and some sample calculations are presented in the next section.

4.1 Basic Method and Definitions

If $P(C,t)$ is the probability that a system will be in configuration $C$ at time $t$, one can write the following master equation for the time derivative of $P(C,t)$:
\[ \partial_t P(C,t) = \sum_{C'} \{ w[C' \rightarrow C] P(C',t) - w[C \rightarrow C'] P(C,t) \}, \]  
\hspace{1cm} (4.1)

where the sum is over all other possible configurations \( C' \) and \( w \)'s are rate functions. For example, \( w[C' \rightarrow C] \) is transition probability per unit time that configuration \( C' \) will change to \( C \). The two-point correlation function \( G \) is the average correlation between two spins, with the average taken over all possible system configurations. Due to translational invariance, \( G \) can be defined using only the displacement vector \( r \) between two spins \( \sigma_0 \) and \( \sigma_r \):

\[ G(r,t) = \langle \sigma_0 \sigma_r \rangle = \sum_C \sigma_0 \sigma_r P(C,t). \]  
\hspace{1cm} (4.2)

The time derivative of \( G(r,t) \) can be expressed in terms of spins and rate functions. The high temperature expansion relies on the fact that the rate functions can be expanded in a Taylor series when \( K = J/(k_B T) \) is small, producing a relatively simple rate to first order. Each \( \partial_t G(r) \) generates an equation involving \( K, \alpha, \epsilon \equiv e^{-E/T} \), and various other correlation functions. Assuming steady state implies \( G(r,t) = G(r) \), so that \( \partial_t G(r,t) = 0 \). These calculations relate to critical temperatures because each \( G(r) \) is a Fourier transform of structure factors. The set of equations involving correlation functions can be converted to a set of equations involving structure factors, which can then be solved. For non-conserved systems, the critical temperature corresponds to the temperature where the magnetic susceptibility \( S(0,0) \) diverges. Some modifications must be made here because of the zero magnetization (half filling) condition. Thus an estimate of the critical temperature will be generated. The solution is obtained first for infinite systems. It does not have the accuracy desired, so the method is then modified to treat finite systems.

### 4.2 Detailed Calculations

#### 4.2.1 Obtaining \( G \)'s

We first derive equations for \( \partial_t G(r) \) using essentially the method of [18]. It can be shown that

\[ \partial_t G(r,t) = \partial_t \langle \sigma_0 \sigma_r \rangle = \sum_{a,b} \langle \sigma_0 \sigma_r (\sigma_a \sigma_b - 1) w(a,b) \rangle, \]  
\hspace{1cm} (4.3)

where the sum is over nearest neighbor sites \( a \) and \( b \) such that \( a \) is either \( 0 \) or \( r \) and \( b \) is a nearest neighbor of \( a \) other than \( 0 \) or \( r \). \( w(a,b) \) refers to the rate (probability) for exchanging the spins at sites \( a \) and \( b \). The sum can be easily divided into terms in which the \( a-b \) bond lies in the field direction and those in which the \( a-b \) bond lies transverse to the field direction. Then the
rate separates into the rate \( w || \) for exchanges in the field direction and the rate \( w _ \perp \) for exchanges in the transverse direction. Defining \( \beta \equiv 1/T \), expanding in powers of \( \beta \), and keeping terms up to first order gives

\[
w _ \perp = \begin{cases} 
1 & \Delta \mathcal{H} < 0 \\
\exp[-\beta \Delta \mathcal{H}] & \Delta \mathcal{H} > 0
\end{cases}
\approx 1 - \frac{1}{2} \beta [\Delta \mathcal{H} + |\Delta \mathcal{H}|] . \tag{4.4}
\]

To simplify \( w || \), we make the additional assumption that \( E > \Delta \mathcal{H} \) always so that up spins will move along \( E \) with probability 1 and will have their probability of moving against \( E \) suppressed. Then, recalling that the drive is in the negative \( x \)-direction,

\[
w || = \begin{cases} 
1 & \Delta \mathcal{H} + E \delta x < 0 \\
\exp[-\beta (\Delta \mathcal{H} + E \delta x)] & \Delta \mathcal{H} + E \delta x > 0
\end{cases}
\]

along \( E \) \hspace{1cm} \text{(4.5)}

\[
= \begin{cases} 
1 & \text{against } E
\end{cases}
\]

\[
= \frac{1}{4} (\sigma _ r - \sigma _ {r-k} + 2) + \frac{1}{4} (\sigma _ {r-k} - \sigma _ r + 2) \exp[-\beta (\Delta \mathcal{H} + E)]
\approx \frac{1}{4} (\sigma _ r - \sigma _ {r-k} + 2) + \frac{1}{4} (\sigma _ {r-k} - \sigma _ r + 2) (1 - \beta \Delta \mathcal{H}) \epsilon,
\]

where \( \sigma _ r \) and \( \sigma _ {r-k} \) are the two spins being exchanged. The first term in the last line of Equation 4.5 is present even in the \( E = \infty \) case, while the second will be nonzero only for finite drives. These facts lead to a decomposition of \( \partial _ t G(r) \) of the form

\[
\partial _ t G(r, t) = A ||_{E=\infty} + \epsilon \tilde{A} || , \tag{4.6}
\]

in which each \( A \) term involves summation of \( \langle \sigma _0 \sigma _r (\sigma _0 \sigma _b - 1)w(a, b) \rangle \) over parallel only or transverse only a-b bonds. These \( A \)'s and hence \( \partial _t G(r) \) can be determined explicitly for all \( r = (x, y) \), since the cases for which \( |x| + |y| > 2 \) can be all expressed in a single equation. Only a small number of cases in which \( r \) is small must be treated separately.

Several properties of correlations are used in simplifying \( A \)'s. The average of a single spin is 0 due the zero magnetization (half filling) condition. A spin times itself is 1. Thus \( G(0, 0) = 1 \). Correlations other than \( G(0, 0) \) are 0 to zero order in \( \beta \). This property holds because at infinite temperature (\( \beta = 0 \)), the steady state probability distribution is uniform. Three-point correlation functions can be neglected to first order in \( \beta \). By symmetry and translational invariance, \( G(x, y) \) is even in both \( x \) and \( y \).

A brief sample calculation of \( \tilde{A} || \) for \( G(1, 0) \) is presented here. For lattice sites labeled as in Figure 16,

\[
\tilde{A} || = \langle \sigma _0 \sigma _r (\sigma _0 \sigma _b - 1) \tilde{w} || (0, h) \rangle + \langle \sigma _0 \sigma _r (\sigma _r \sigma _d - 1) \tilde{w} || (r, d) \rangle, \tag{4.7}
\]

where for example

\[
\tilde{w} || (0, h) \equiv \frac{1}{4} (\sigma _h - \sigma _0 + 2) (1 - \beta \Delta \mathcal{H}(0, h))
\]

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The energy change upon exchange of the spins at 0 and at $h$ is
\[ \Delta \mathcal{H}(0, h) = -(\sigma_0 - \sigma_h) \{ J_{\parallel} \sigma_1 + J_{\perp} \sigma_n + J_{\perp} \sigma_g - (J_{\parallel} \sigma_r + J_{\perp} \sigma_b + J_{\perp} \sigma_f) \}, \]
and $\Delta \mathcal{H}(r, d)$ is similar in form. After substitution into Equation 4.7 and the aforementioned simplifications, $\hat{A}_{\parallel}$ becomes
\[ \hat{A}_{\parallel} = G(2, 0) - G(1, 0) + 2\beta J_{\parallel}, \]

Figure 16. Lattice site names for sample calculation of $\hat{A}_{\parallel}$ for $G(1, 0)$.

Similar analyses for the other $A$'s lead to the following linear set of equations valid to first order in $K_{\parallel}, K_{\perp}$ (with the $t$ argument suppressed for simplicity):

\[ \partial_t G(1, 0) = 2 [G(1, 1) + G(1, -1) - 2G(1, 0)] + (1 + \epsilon) [G(2, 0) - G(1, 0)] + 2K_{\parallel} (2 + \epsilon) \]
\[ \partial_t G(0, 1) = 2 [G(0, 2) - G(0, 1)] + (1 + \epsilon) [G(1, 1) + G(-1, 1) - 2G(0, 1)] + 2K_{\perp} (1 + 2\epsilon) \]
\[ \partial_t G(1, 1) = 2 [G(1, 2) + G(1, 0) - 2G(1, 1)] + (1 + \epsilon) [G(2, 1) + G(0, 1) - 2G(1, 1)] \] (4.8)
\[ -2K_{\parallel} - 2K_{\perp} \]
\[ \partial_t G(2, 0) = 2 [G(2, 1) + G(2, -1) - 2G(2, 0)] + (1 + \epsilon) [G(3, 0) + G(1, 0) - 2G(2, 0)] - 2K_{\parallel} \]
\[ \partial_t G(0, 2) = 2 [G(0, 3) + G(0, 1) - 2G(0, 2)] + (1 + \epsilon) [G(1, 2) + G(-1, 2) - 2G(0, 2)] - 2K_{\perp} \]

and, for all $(x, y)$ such that $|x| + |y| > 2$:

\[ \partial_t G(x, y) = 2 [G(x, y + 1) + G(x, y - 1) - 2G(x, y)] + (1 + \epsilon) [G(x + 1, y) + G(x - 1, y) - 2G(x, y)]. \] (4.9)

### 4.2.2 An integral solution for infinite system sizes

To obtain the steady state equations (i.e., those with no time dependence), we set the left sides of Equations 4.8 and 4.9 to 0:

\[ 0 = 2 [G(1, 1) + G(1, -1) - 2G(1, 0)] + (1 + \epsilon) [G(2, 0) - G(1, 0)] + 2K_{\parallel} (2 + \epsilon) \]
0 = 2[G(0, 2) - G(0, 1)] + (1 + \epsilon) [G(1, 1) + G(-1, 1) - 2G(0, 1)] + 2K_\perp (1 + 2\epsilon)
0 = 2[G(1, 2) + G(1, 0) - 2G(1, 1)] + (1 + \epsilon) [G(2, 1) + G(0, 1) - 2G(1, 1)]
-2K_\parallel - 2\epsilon K_\perp
0 = 2[G(2, 1) + G(2, -1) - 2G(2, 0)] + (1 + \epsilon) [G(3, 0) + G(1, 0) - 2G(2, 0)] - 2\epsilon K_\parallel
0 = 2[G(0, 3) + G(0, 1) - 2G(0, 2)] + (1 + \epsilon) [G(1, 2) + G(-1, 2) - 2G(0, 2)] - 2K_\perp

and, for all \((x, y)\) such that \(|x| + |y| > 2:\)
0 = 2 [G(x, y + 1) + G(x, y - 1) - 2G(x, y)]
+ (1 + \epsilon) [G(x + 1, y) + G(x - 1, y) - 2G(x, y)].

Next we follow the method of [17] to solve these equations. The only difference in this analysis is the presence of both \(K_\parallel\) and \(K_\perp\) so that anisotropic interactions are described. The solution to Equations 4.10 and 4.11 can be found most easily in Fourier space. Structure factors are Fourier transforms of correlation functions:

\[
S(k, p) = \sum_{x,y}^\infty G(x, y) \exp[-i(kx + py)].
\]

\(S(k, p)\) will be real because \(G\) is even by symmetry. To zero order in \(K\) (infinite temperature or noninteracting particles), the distribution of states is known to be uniform. Hence the zero order solution is known:

\[
G(0, 0) = 1
\]
\[
G(x, y) = 0 \text{ for } (x, y) \neq (0, 0),
\]

This gives \(S(k, p)\) to zero order in \(K:\)

\[
S(k, p) = 1 \equiv \tilde{S}.
\]

We define a first order correction \(\tilde{S}\) to \(S\) so that to first order in \(K\),

\[
S = \tilde{S} + \tilde{S}
\]

(4.13)

The correlation functions in Equations 4.10 and 4.11 are first order in \(K\) and so are inverse Fourier transforms of \(\tilde{S}\). We define the notation

\[
\int \equiv \frac{1}{(2\pi)^2} \int_{-\pi}^{+\pi} dk \int_{-\pi}^{+\pi} dp
\]

for convenience and can then write

\[
G(x, y) = \int \tilde{S}(k, p) \exp[i(kx + py)] \text{ for } (x, y) \neq (0, 0).
\]

This result is substituted into Equations 4.10 and 4.11, and some simplification can be done. The simplification relies on the fact that \(\tilde{S}(k, p)\) is real and
even (which can be seen by observing Equations 4.12 and 4.13 and recalling that \( G(x, y) \) is even). Simplification of the first equation in 4.10 is presented here in some detail. The calculation is as follows:

\[
0 = 2 \int \tilde{S} \left[ e^{i(k+p)} + e^{i(k-p)} - 2e^{ik} \right] + \left( 1 + \epsilon \right) \int \tilde{S} \left[ e^{2ik} - e^{ik} \right] + 2K_{\parallel}(2 + \epsilon)
\]

\[
= \int \tilde{S}e^{ik} \left[ 4(\cos p - 1) + (1 + \epsilon)(e^{ik} - 1) \right] + 2K_{\parallel}(2 + \epsilon)
\]

\[
= \int \tilde{S}e^{ik} \left[ 4(\cos p - 1) + (1 + \epsilon)(2\cos k - 2) \right] + (1 + \epsilon) \int \tilde{S}(e^{ik} - 1) + 2K_{\parallel}(2 + \epsilon)
\]

\[
= -\int \tilde{S}e^{ik} \left[ 4(1 - \cos p) + 2(1 + \epsilon)(1 - \cos k) \right] + (1 + \epsilon) \int \tilde{S}(\cos k - 1) + 2K_{\parallel}(2 + \epsilon).
\]

For greater ease in writing such results, we define

\[
\Delta(k, p) = 4(1 - \cos p) + 2(1 + \epsilon)(1 - \cos k).
\]

Using similar manipulations on the rest of Equations 4.10 and 4.11, we obtain

\[
\int \tilde{S} \Delta e^{ik} + (1 + \epsilon) \int \tilde{S}(1 - \cos k) = 2K_{\parallel}(2 + \epsilon) \quad (4.15)
\]

\[
\int \tilde{S} \Delta e^{ip} + 2 \int \tilde{S}(1 - \cos p) = 2K_{\perp}(1 + 2\epsilon)
\]

\[
\int \tilde{S} \Delta e^{i(k+p)} = -2K_{\parallel} - 2\epsilon K_{\perp}
\]

\[
\int \tilde{S} \Delta e^{2ik} = -2K_{\parallel}
\]

\[
\int \tilde{S} \Delta e^{2ip} = -2K_{\perp},
\]

similar equations for negative \( x \) and \( y \) (since \( \tilde{S} \) and \( \Delta \) are even in \( k, p \)), and

\[
\int \tilde{S} \Delta e^{i(kx+py)} = 0 \text{ for all } (x, y) \text{ such that } |x| + |y| > 2. \quad (4.16)
\]

To extract an equation for \( \tilde{S} \) from Equations 4.15 and 4.16, we use the fact that the functions \( 1/(2\pi) \exp(i(kx + py)) \) form a complete orthonormal set. That is,

\[
\sum_{x,y} \frac{1}{2\pi} e^{i(kx+py)} \frac{1}{2\pi} e^{i(lx+ly)} = \delta(k-l)\delta(p-q). \quad (4.17)
\]

Hence the following procedure will produce an equation for \( \tilde{S} \): multiply both sides of Equations 4.15 and 4.16 by \( e^{i(kx+py)} \) (with the appropriate \( x \) and \( y \) for each equation) and sum over all \( x, y \). The additional terms on the left side in
the first two lines of 4.15 do not fit into this approach, but we will treat them
for the moment as unknown \( \epsilon \)-dependent coefficients,

\[
I_1 \equiv \int \hat{S}(1 - \cos k) \quad (4.18)
\]

\[
I_2 \equiv \int \hat{S}(1 - \cos p),
\]

and put them on the right hand side of 4.15. To use the completeness relation,
we need an equation for \( x = y = 0 \), but this is just

\[
\int \hat{S} \Delta = \int \hat{S} [4(1 - \cos p) + 2(1 + \epsilon)(1 - \cos k)] = 2(1 + \epsilon)I_1 + 4I_2.
\]

Now we use the completeness relation (Equation 4.17) to obtain

\[
\hat{S}(k, p) = L(k, p)/\Delta(k, p), \quad (4.19)
\]

where \( L \) is the sum of terms from the right hand sides, namely

\[
L(k, p) \equiv 2I_1(1 + \epsilon)(1 - \cos k) + 4I_2(1 - \cos p) + 4[\epsilon(1 - \cos k) (K_{||} + 2K_{||} \cos k + 2K_{\perp} \cos p)
+ (1 - \cos p) (K_{\perp} + 2K_{||} \cos k + 2K_{\perp} \cos p)].
\]  (4.20)

Equation 4.19 is only an implicit equation for \( \hat{S} \), since the \( I_1 \) and \( I_2 \) terms on
the right side depend on \( \hat{S} \). To obtain an explicit solution, we need to find the
\( I \)'s. There are two unknowns, so we need two linearly independent equations.
The first is found by substituting the result for \( \hat{S} \) (Equation 4.19) into the
definition of \( I_1 \) (Equation 4.18). This yields

\[
0 = -I_1 + \int \frac{L}{\Delta}(1 - \cos k) = M_{11}I_1 + M_{12}I_2 + N_1
\]

where

\[
M_{11} \equiv -1 + 2(1 + \epsilon) \int \frac{(1 - \cos k)^2}{\Delta(k, p)}
\]

\[
M_{12} \equiv 4 \int \frac{(1 - \cos k)(1 - \cos p)}{\Delta(k, p)} \quad (4.21)
\]

\[
N_1 \equiv 4 \int [\epsilon(1 - \cos k)^2 (K_{||} + 2K_{||} \cos k + 2K_{\perp} \cos p)
+ (1 - \cos k)(1 - \cos p) (K_{\perp} + 2K_{||} \cos k + 2K_{\perp} \cos p)]/\Delta(k, p).
\]

For the isotropic system, the second equation of 4.18 is not linearly independent
of the first, a result of a symmetry under \((k, p)\) exchange [17]. However,
an additional equation involving $I_1, I_2$ can be found because $G(0, 0) = 1$ both exactly and to zero order in $K$. Thus $S = \tilde{S} = 1$, so

$$0 = \int \tilde{S}(k, p) = \int \frac{L(k, p)}{\Delta(k, p)} = M_{21}I_1 + M_{22}I_2 + N_2$$

where

$$M_{21} \equiv 2(1 + \epsilon) \int \frac{(1 - \cos k)}{\Delta(k, p)}$$

$$M_{22} \equiv 4 \int \frac{(1 - \cos p)}{\Delta(k, p)}$$

$$N_2 \equiv 4 \int \left[ \epsilon(1 - \cos k) \left( K_{\parallel} + 2K_{\parallel} \cos k + 2K_{\perp} \cos p \right) \\
+ (1 - \cos p) \left( K_{\perp} + 2K_{\parallel} \cos k + 2K_{\perp} \cos p \right) \right] / \Delta(k, p).$$

The integrals in Equations 4.21 and 4.22 are finite because at $(k, p) = (0, 0)$ when the denominators is 0, the numerators are all 0 as well. The explicit solution for the $I$'s follows by inverting the matrix $M$:

$$I_m = -M_{mn}^{-1}N_n.$$

Note that $\tilde{S}$ is $O(K)$ as expected, since each $N_n$ carries a factor of $K$.

We need not resort to numerical approximations at this point, since the integrals in Equations 4.21 and 4.22 can be calculated analytically. The integrals are of the form

$$R_{ij} = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \, dk \int_{-\pi}^{\pi} \, dp \frac{(1 - \cos k)^i(1 - \cos p)^j}{A(1 - \cos k) + B(1 - \cos p)}$$

for $A = 2(1 + \epsilon), B = 4$. Even $N_1, N_2$ have this form:

$$N_1 = 4 \left[ \epsilon(3K_{\parallel} + 2K_{\perp})R_{00} - 2\epsilon K_{\parallel} R_{10} - 2(\epsilon K_{\parallel} + K_{\parallel})R_{01} + (2K_{\parallel} + 3K_{\perp})R_{11} - 2K_{\perp}R_{12} \right]$$

$$N_2 = 4 \left[ \epsilon(3K_{\parallel} + 2K_{\perp})R_{10} - 2\epsilon K_{\parallel} R_{00} - 2(\epsilon K_{\parallel} + K_{\parallel})R_{11} + (2K_{\parallel} + 3K_{\perp})R_{01} - 2K_{\perp}R_{02} \right].$$

We actually need compute only $R_{00}$ because the other $R_{ij}$ can be determined from the identities

$$AR_{00} + BR_{01} = \int \frac{\Delta(k, p)}{\Delta(k, p)} = 1$$

$$AR_{00} + BR_{11} = \int \frac{(1 - \cos k)\Delta(k, p)}{\Delta(k, p)} = 1$$

$$AR_{11} + BR_{02} = \int \frac{(1 - \cos p)\Delta(k, p)}{\Delta(k, p)} = 1$$

$$AR_{00} + BR_{21} = \int \frac{(1 - \cos k)^2\Delta(k, p)}{\Delta(k, p)} = \frac{3}{2}.$$
\[ AR_{q_1} + BR_{q_2} = \int \frac{(1 - \cos k)(1 - \cos p)\Delta(k, p)}{\Delta(k, p)} = 1 \]
\[ AR_{q_2} + BR_{q_3} = \int \frac{(1 - \cos p)^2 \Delta(k, p)}{\Delta(k, p)} = \frac{3}{2} \]

By integrating over \( p \) and making the substitutions \( z = A/B \) and \( 2t = 1 - \cos k \), we can show that the \( R_{q_i} \) are essentially hypergeometric functions [19]:

\[
R_{q_0} = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk \int_{-\pi}^{\pi} dp \frac{(1 - \cos k)^i}{A(1 - \cos k) + B(1 - \cos p)}
\]
\[
= \frac{1}{2\pi B} \int_{-\pi}^{\pi} \frac{(1 - \cos k)^i}{\sqrt{z(1 - \cos k) + 1}} dk
\]
\[
= \frac{1}{\pi B \sqrt{z}} \int_{0}^{\pi} \frac{(1 - \cos k)^{-1/2}}{\sqrt{z(1 - \cos k) + 2}} dk
\]
\[
= \frac{1}{\pi B \sqrt{z}} \int_{0}^{1} t^{i-1}(1 - t)^{-1/2}(1 + zt)^{-1/2} dt
\]
\[
= \frac{1}{\pi B \sqrt{z}} \frac{\Gamma(1/2)\Gamma(i)}{\Gamma(i + 1/2)} F \left( \frac{1}{2}, i + \frac{1}{2}; z \right).
\]

The hypergeometric functions can be obtained from tables. Thus the \( I \)'s and then \( \tilde{S} \) can be calculated exactly. However, the explicit solutions are quite lengthy and not particularly enlightening, so they will not be quoted here.

Hence the full solution for \( S(k, p) \) can be found to first order in \( K \):
\[
S = \tilde{S} + \frac{L}{\Delta} + O(K^2).
\]

If the system were nonconservative and we had the exact solution for \( S(k, p) \), we could easily locate \( T_r \) by the divergence of the susceptibility \( S(0, 0) \). However, the zero magnetization (half filling) condition for this system fixes \( S(0, 0) = 0 \). Thus we must instead look at \( \lim_{(k, p) \to (0, 0)} S(k, p) \). However, further subtleties arise. The structure factor for the driven system has a discontinuity at the origin. In particular, \( \lim_{p \to 0} S(0, p) \neq \lim_{k \to 0} S(k, 0) \). This can be seen easily from a series expansion in \( k, p \) to second order. Rearrangement and simplification produces
\[
S(k, p) = \frac{n_{||} k^2 + n_{\perp} p^2}{\tau_{||} k^2 + \tau_{\perp} p^2 + O(k^4, k^2 p^2, p^4)}
\]

where
\[
\tau_{||} = (1 + \epsilon)(1 - I_1) - 6\epsilon K_{\perp} - 4\epsilon K_{\perp} \tag{4.24}
\]
\[
\tau_{\perp} = 2(1 - I_2) - 4K_{\|} - 6K_{\perp}
\]

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\[ n_\parallel = 1 + \epsilon \]
\[ n_\perp = 2 \]

We note that for large fields, only \( S(0, p) \) should diverge as \( (k, p) \to (0, 0) \) because the only ordered phase is aligned parallel to the field. Thus it seems reasonable to look for the divergence of \( S(k, p) \) via \( \lim_{p \to 0} S(0, p) \). Another problem arises: in a high temperature expansion, where only a finite number of terms are summed, \( S(k, p) \) will never diverge. Thus we will instead look for the zero of \( S^{-1} \) to first order. This is equivalent to finding the zero of \( \tau_\perp \).

The solution for the critical temperature is
\[
T_c(\alpha, E) = \frac{1}{k_B} \left( \frac{I_2}{\beta} + 2J_\parallel + 3J_\perp \right). \tag{4.25}
\]

\( I_2 \) is proportional to \( \beta \), and \( I_2 / \beta \) depends on \( \beta \) only through \( \epsilon \). Thus at \( E = 0 \) \( (\epsilon = 1) \) and \( E = \infty \) \( (\epsilon = 0) \), the solution for \( T_c(\alpha, E) \) can be computed by simple substitution. Results are discussed in detail below. However, it should be noted briefly at this point that the approximate \( T_c(\alpha, E) \) generated by this method does not decrease monotonically with \( E \).

4.2.3 A summation solution for finite system sizes

Hoping to obtain better agreement with Monte Carlo simulation results, we modify the above method for finite systems. Integrals are replaced by finite sums. The relationships between the correlation function and the structure factors become

\[
G(x, y) = \frac{1}{L_x L_y} \sum_{l=-L_x-1}^{L_x-1} \sum_{m=-L_y-1}^{L_y-1} S(k, p) e^{i(kx+py)}
\]

where
\[
k = \frac{2\pi l}{L_x}, \quad p = \frac{2\pi m}{L_y}
\]

\[
S(k, p) = \sum_{x=-L_x-1}^{L_x-1} \sum_{y=-L_y-1}^{L_y-1} G(x, p) e^{-i(kx+py)}.
\]

As before, we break \( S(k, p) \) into a zero order solution \( \bar{S} \) and a first order correction \( \tilde{S} \). Now, however, the correlation between two different spins at \( \beta = 0 \) is a small negative number because of the finite system size. This means

\[
G(0, 0) = 1
\]
\[
\bar{G}(x, y) = g \text{ for } (x, y) \neq (0, 0),
\]

where \( g \equiv -1/(L_x L_y - 1) \). Then

\[
\tilde{S}(k, p) = (1 - g)(1 - \delta_{k,0}\delta_{p,0}).
\]
We substitute $G(x, y)$ from 4.26 into the set of linear equations involving $G$'s, Equations 4.10 and 4.11. $\tilde{S}$ should solve the equations to zero order in $K$, and the unknown first order correction $\tilde{S}$ should also solve them. $S(0, 0) = 0$ and $\tilde{S}(0, 0) = 0$ implies $\tilde{S}(0, 0) = 0$, so we do not need to include the $(k, p) = (0, 0)$ term of the summation in Equation 4.26. For convenience, we define the notation

$$\int' \equiv \sum_{l=-(L_x-1)/2}^{(L_x-1)/2} \sum_{m=-(L_y-1)/2}^{(L_y-1)/2}$$

except the $(l, m) = (0, 0)$ term.

Then the substitution of $G(x, y)$ in terms of $\tilde{S}$ yields a set of equations identical to 4.15 and 4.16 except for the occurrence of $\int'$ instead of $\int$. (Simplification relies on the fact that $\tilde{S}$ is even.)

To extract an equation for $\tilde{S}$, we multiply by $\exp[-i(rx + qy)]$ and use the completeness relation

$$\sum_{x=-(L_x-1)/2}^{(L_x-1)/2} \sum_{y=-(L_y-1)/2}^{(L_y-1)/2} e^{i(kx+py)} e^{-i(rx+qy)} = \delta_{k, x} \delta_{p, y}.$$

The calculation proceeds just as in the infinite system case except that $\int'$ appears instead of $\int$ everywhere. $I_i, M_{ij},$ and $N_j$ are defined similarly to before, and the solution is $I_i = -M_{ij}^{-1} N_j$. The $R_{ij}$'s are now finite sums which can be computed to arbitrary precision on a computer.

$S$ can thus be calculated. The finite system analog to Equation 4.24 is

$$S(k, p) = \frac{n_{||} k^2 + n_{\perp} p^2}{\tau_{||} k^2 + \tau_{\perp} p^2 + O(k^4, k^2 p^2, p^4)}$$

where

$$\begin{align*}
\tau_{||} &= (1 + \epsilon)(1 - g - I_1) - 6\epsilon K_{||} - 4\epsilon K_{\perp} \\
\tau_{\perp} &= 2(1 - g - I_2) - 4K_{||} - 6K_{\perp} \\
n_{||} &= (1 + g)^2 (1 + \epsilon) \\
n_{\perp} &= 2.
\end{align*}$$

(4.27)

Finding the zero of $S^{-1}$ in the limit as $p \to 0$ yields a critical temperature of

$$T_c(\alpha, E) = \frac{1}{k_B} \frac{1}{1 - g} \left( \frac{I_2}{\beta} + 2I_{||} + 3I_{\perp} \right).$$

(4.28)

4.3 Series Expansion Results and Discussion

At $\alpha = 1$, Equation 4.25 reproduces the result of [17]: $T_c(1, 0) = 4, T_c(1, \infty) = 4.64$. So, as mentioned previously, the high temperature expansion predicts
qualitatively the monotonic increase of \( T_c(1,E) \). Since this result runs counter to original intuition, the series expansion certainly has some value. However, it does not reproduce the result found in Monte Carlo simulations that \( T_c(\alpha, \infty) \) decreases monotonically with \( \alpha \). Changing units by dividing by 4 so that the series expansion \( T_c(1,0) = 1 \), we obtain the curves in Figure 17 for the anisotropic system. Although the \( \alpha > 1 \) side of \( T_c(\alpha, \infty) \) is slightly lower than the \( \alpha < 1 \) side, \( T_c \) still increases with \( \alpha \).

![Phase diagram predicted by high temperature expansion for an infinite system](image_url)

**Figure 17.** Critical temperatures predicted by high temperature expansion for infinite systems at equilibrium and with infinite drive.

Critical temperature results for two finite sized systems with infinite drive are shown in Figure 18, along with the infinite system result for comparison. \((E = 0\) results are not displayed because they are identical for finite and infinite systems in this calculation.) Temperatures are again rescaled so that \( T_c(1,0) = 1 \). Odd values of \( L_x \) and \( L_y \) must be used because of the presence of \((L_x - 1)/2\) and other such limits in the summations. The \( 29 \times 29 \) system ought to display a phase diagram similar to the one that Monte Carlo studies found for a \( 30 \times 30 \) system, but it does not. Both of the finite systems have a phase diagram very similar to the infinite one in the high temperature expansion. It is interesting to note, though, that \( T_c(\alpha, \infty) \) increases with system size in the high temperature expansion, just as it did in Monte Carlo simulations.
Figure 18. Critical temperatures predicted by high temperature expansion for $9 \times 9$, $29 \times 29$, and infinite systems with infinite drives.

So the series expansion fails to reproduce all of the interesting qualitative characteristics of the driven anisotropic Ising model phase diagram. The expansion assumed high temperatures, and we had extrapolate back down to lower temperatures to extract information about the critical temperature. Thus it is understandable that the high temperature expansion method would have only partial success in making predictions about the phase diagram, especially since this calculation was only to first order. Ideally, we would extend the above work to higher order expansions. However, it is prohibitively difficult to compute even the second order terms of the expansion. Thus it appears that high temperature expansions will have only limited value in providing insight into complex nonequilibrium systems. Clearly, other approaches are needed. The dynamic mean field method [20] could be extended to our system and might produce more accurate results.
Chapter 5

Conclusions

Through Monte Carlo simulations, a fairly accurate phase diagram was computed for the 30×30 anisotropic driven Ising lattice gas. Preliminary studies of the effect of system size suggest that key features of this phase diagram will survive in the thermodynamic limit. In the process of determining the phase diagram, we developed a new technique for locating first order transitions. This method involves studying the “energy landscape” in the vicinity of the saddle point between two ordered phases. At the temperature where it was compared with the standard method of hysteresis loop analysis, the saddle point method produced fairly consistent results. It should be applicable to locating first order transition lines in other nonequilibrium systems.

The phase diagram, in the three dimensions of $\alpha, T, E$, was found to be quite complex. Several of its properties were unexpected, such as the monotonic decrease of $T_c(\alpha, \infty)$ with $\alpha$. It is hoped that further study will lead to a better understanding of why driven systems behave as they do. One of the more interesting observations of these studies was the presence of “stringy states” at large $\alpha$ and $E$ values. The system exhibits long range order in the field direction but not in the transverse direction. Preliminary investigations show these stringy states to persist in systems as large as 90×90. We hypothesize that the drive may cause a new phase to occur between the completely ordered single strip phase and the completely disordered phase. Our observations so far have been consistent with this idea. Further study is needed of larger systems. We also found unusual behavior in the frequency distributions of structure factors for these systems, which could be related to the presence of stringy states. More detailed analysis is needed to determine the connection.

The phase diagram found by Monte Carlo techniques provided a baseline against which high temperature expansion results were compared. Future theoretical predictions will be tested by comparing them with this phase diagram.
as well. The high temperature expansion had only limited success in predicting the interesting properties of the phase diagram. It failed to predict the monotonically decrease of $T_c(\alpha, \infty)$ with $\alpha$. Dynamic mean field techniques [20] may have more success in predicting the phase diagram of the anisotropic system. Certainly other methods must be used if we are to understand from theoretical principles the behavior of this system.

This work has contributed to the subject of nonequilibrium statistical mechanics, partly by providing new information and partly by raising new questions. It is hoped that future studies built off these will lead to a better understanding of the complex behavior of nonequilibrium systems.
Bibliography


[13] The occurrence of a first order transition is dependent on the particular boundary conditions we have chosen. Were the boundaries outside the lattice all up spins, for example, the system would not have a first order transition.


Appendix A

Sample C++ Source Code

/****************************
This program, ising27, evolves a 2D Li x Lj lattice of driven up spins
and down spins over time using Monte Carlo techniques. It computes a
correlation function between spins differing by up to Li/2 units in the
i direction and spins differing by up to Lj/2 units in the j direction.
At the end, it outputs the average of each of the correlation functions.
It collects structure factor data and at the end outputs average
structure factors S(k,p) for k and p from 0 to 6. It also outputs the
variance in S(0,1) and S(1,0). It outputs the ratio
R, a time average of instantaneous R=(L/2)*G(L/2,0)/S(0,1) values, and
RFA, the R value computed from average G and S. It also computes and
outputs a histogram of the number of times columns with each possible
number of up spins are observed. At the command prompt, type
ising27 inputfilename outputfilename
Coordinate conventions: i is row and j is column, and the origin is at
the upper left. The field points up; i.e., it drives up spins (+1) upward
and down spins (-1) downward.

Input file format:
initial config (r for random, v for vertical strip, h for horizontal strip,
s for X shape (St. Andrew's cross), or l for L shape, but
use s and l for different system sizes only after checking
that they preserve the half filling condition)
alpha (anisotropy parameter)
temperature (in units so that Tc(E=0,alpha=1) is 1)
field (in units of J/kB)
number of Monte Carlo steps to run
seed for random number generator (a negative integer)

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This program is not affected by the Y2K problem.
Leah Belinda Shaw, fall 1998
(Column density histogram-related functions were written by Jean Hager.
*******************************************************************************/

#include <fstream.h>  //for file input and output
#include <math.h>  //for calculating exponentials, sines, and cosines
#include <iomanip.h>  //for formatting of output

const double PI=3.141592653589;  //some compilers need this defined;
      //others have it built in
const int Li=30;  //number of rows in lattice
const int Lj=30;  //number of columns in lattice
const int Ci=int((Li+1)/2)+1;
const int Cj=int((Lj+1)/2)+1;
const int C=6;  //structure constant array will go from 0 to 5
const int DISCARD=100000;  //number of initial MCS’s to discard
      //before starting to take averages
const int INTERVAL=200;  //number of MCS’s between taking data points

typedef int Grid[Li][Lj];  //an Li x Lj array
typedef double StructFact[C][C];  //CxC array of structure factors
typedef float Correli[Ci];  //array of correlation functions in i direction
typedef float Correlj[Cj];  //array of correlation functions in j direction
typedef int Hist[Li+1];  //histogram array of number of columns with i
      //up spins
enum Bondtype {HORIZONTAL, VERTICAL};

float ran2(long *idum);  //random number generator
void initialize(Grid, char, long*);  //initializes the lattice to selected
      //configuration
void picture(Grid, ofstream&);  //prints a picture of the lattice to output
      //file
void printF(StructFact, ofstream&);  //prints the structure factor array to
      //output file
void exchange(int&, int&);  //exchanges two array elements
float updatedata(Grid, StructFact, double&, double&, int&);  //collects
      //structure factor and variance data,  
      //adding new values to running sums,  
      //and returns instantaneous S(0,1)
float updatecorr(Grid, Correli, Correlj, ofstream&);  //collects correlation
      //function data, adding new values to
      //running sums, and returns
      //instantaneous G(L/2,0)
void cleardist(Hist); //sets all elements of column density histogram to
//zero
void update_hist_data(Grid, Hist, ofstream&); //collects column density
//histogram data, adding new values to running sums
void printH(Hist, ofstream&); //prints column density histogram
//values and an ASCII schematic of histogram to
//output file

void main(int argc, char *argv[])
{
  Grid lattice; //declare the lattice
  StructFact F={0.0}; //declare the structure factor array and
  //initialize it with 0's. F[i][j] is structure factor for
  //k=(1*2*PI/Li, j*2*PI/Lj)
  double Fsqr10=0.0; //average square of structure factor for
  //k=(2*PI/Li, 0)
  double Fsqr01=0.0; //average square of structure factor for
  //k=(0, 2*PI/Lj)
  Correli corri={0.0}; //declare the i direction correlation function and
  //initialize it with 0's. corri[n] is correlation function
  //G(n,0)
  Correlj corrj={0.0}; //declare the j direction correlation function and
  //initialize it with 0's. corri[n] is correlation function
  //G(n,0)
  Hist distribution; //declare the column density frequency histogram
  cleardist(distribution); //initialize histogram with 0's
  float R=0; //will be running sum of Li*Lj*G(Lx/2,0)/S(0,1)

  ifstream input; //input file stream
  input.open(argv[1]); //open input file: 1st string typed after
  //program name
  ofstream output; //output file stream
  output.open(argv[2]); //open output file: 2nd string typed after
  //program name

  char intialtype; //configuration to initialize to
double alpha; //anisotropy parameter
long inputseed; //input seed for random number generator
double Jperp;
double Jpara;
double T; //temperature in units such that equilibrium isotropic Tc is 1
double E;
int totMCS; //total number of Monte Carlo steps to take

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int numdata=0;     //number of data points taken
double num_avg_hist = 0; // number of averaged histogram data written
    // to file

    /* Start initialization */

    input >> initialtype;

    input >> alpha;
    Jpara=alpha;
    Jperp=1/alpha;

    input >> T;
    double Ti=T;     //store T in original units to output later
    T=T*2.269;       //convert T to units needed to run simulation

    input >> E;

    input >> totMCS;

    input >> inputseed;
    long* seed=&inputseed;
    int inseed=inputseed;     //save initial inputseed to output later

    initialize(lattice, initialtype, seed);

    //output the input values
    output << "initial configuration: " << initialtype << endl;
    output << Li << 'x' << Lj << endl;
    output << "alpha=" << alpha << endl;
    output << "T=" << Ti << endl;
    output << "E=" << E << endl;
    output << totMCS << " Monte Carlo steps" << endl;
    output << "take data every " << INTERVAL << " MCS" << endl;
    output << "discard first " << DISCARD << " MCS" << endl;
    output << "inputseed=" << inseed << endl;

    /* End initialization */

    /* Start Monte Carlo simulation */

    int numMCS;     //count of which MCS the simulation is in
                   for (numMCS=1; numMCS<=totMCS; numMCS++)
    {
        /* Start Monte Carlo step */

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int numbonds; //number of bonds checked in current MCS

for (numbonds=1; numbonds<=2*Lj; numbonds++)
{
    // Choose a random bond between two nearest neighbor spins
    int ran=(int(Li*Lj*2*ran2(seed)))%(Li*Lj*2); //random integer
    //between 0 and 2*Li*Lj-1

    Bondtype bond;

    if (ran<Li*Lj)
        bond=HORIZONTAL;
    else
    {
        bond=VERTICAL;
        ran-=Li*Lj;
    }

    int i1=ran/Lj; //i coordinate of spin to look at
    int j1=ran%Lj; //j coordinate of spin to look at

    /* Start horizontal bond */

    if (bond==HORIZONTAL)
    {
        /*
        horizontal configuration: 
         pU1 pU2
            pl  p1  p2  pR
            pD1 pD2
         with bond between p1 & p2
        */

        int j2=(j1==Lj-1)? 0 : (j1+1); //column after j1

        //if the two spins are different
        if (lattice[i1][j1]!=lattice[i1][j2])
        {
            int iU=(i1==0)? (Li-1) : (i1-1); //row above spins
            int iD=(i1==Li-1)? 0 : (i1+1); //row below spins
            int jL=(j1==0)? (Lj-1) : (j1-1); //column to left of spins
            int jR=(j1==Lj-1)? 0 : (j2+1); //column to right of spins

            int Hperp=0; //negative of energy due to bonds perpendicular
                       //to field (horizontal bonds) (energy component
                       //that will contribute to deltaH)

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//bond p1-pL
if (lattice[i1][j1]==lattice[i1][jL]) Hperp++;
   else Hperp--;

//bond p2-pR
if (lattice[i1][j2]==lattice[i1][jR]) Hperp++;
   else Hperp--;

int Hpara=0; //negative of energy due to bonds parallel to
   //field (vertical bonds) (energy component
   //that will contribute to deltaH)

//bond p1-pU1
if (lattice[i1][j1]==lattice[iU][j1]) Hpara++;
   else Hpara--;

//bond p1-pD1
if (lattice[i1][j1]==lattice[iD][j1]) Hpara++;
   else Hpara--;

//bond p2-pU2
if (lattice[i1][j2]==lattice[iU][j2]) Hpara++;
   else Hpara--;

//bond p2-pD2
if (lattice[i1][j2]==lattice[iD][j2]) Hpara++;
   else Hpara--;

double deltaH=2.*(Hperp*Jperp+Hpara*Jpara); //energy change if
   //spins switch

double prob=exp(-deltaH/T); //probability of the spins switching

if (prob>1.) exchange(lattice[i1][j1], lattice[i1][j2]);
   else if (ran2(seed)<prob)
      exchange(lattice[i1][j1],lattice[i1][j2]);
} }
/* End horizontal bond */

/* Start vertical bond */
else
{
   /*
   * vertical configuration: pU
   */
pL1 p1 pR1
p12 p2 pR2
pD

with bond between p1 & p2

*/

int i2=(i1==Li-1)?0:(i1+1);

//if the two spins are different
if (lattice[i1][j1]!=lattice[i2][j1])
{
    int iU=(i1==0)?(Li-1):(i1-1);
    int iD=(i2==Li-1)?(i2+1):(i2-1);
    int jL=(j1==0)?(Lj-1):(j1-1);
    int jR=(j1==Lj-1)?(j1+1):(j1+1);

    int Hperp=0; //negative of energy due to bonds perpendicular
                 //to field (horizontal bonds) (energy component
                 //that will contribute to deltaH)

    //bond pL1-p1
    if (lattice[i1][j1]==lattice[i1][jL]) Hperp++;
    else Hperp--;

    //bond pL2-p2
    if (lattice[i2][j1]==lattice[i2][jL]) Hperp++;
    else Hperp--;

    //bond p1-pR1
    if (lattice[i1][j1]==lattice[i1][jR]) Hperp++;
    else Hperp--;

    //bond p2-pR2
    if (lattice[i2][j1]==lattice[i2][jR]) Hperp++;
    else Hperp--;

    int Hpara=0; //negative of energy due to bonds parallel to
                 //field (vertical bonds) (energy component
                 //that will contribute to deltaH)

    //bond p1-pU
    if (lattice[i1][j1]==lattice[iU][j1]) Hpara++;
    else Hpara--;

    //bond p2-pD
    if (lattice[i2][j1]==lattice[iD][j1]) Hpara++;

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else Hpara--;

double deltaH=2.*(Hperp*Jperp+Hpara*Jpara); //energy change if
//spins switch

int epsilon;
if (lattice[i1][j1]==1) //positive spin would be moving against
//field
    epsilon=1;
else epsilon=-1; //positive spin would be moving along field

double prob=exp(-(deltaH+epsilon*E)/T); //probability of the
//spins switching

if (prob>1.) exchange(lattice[i1][j1], lattice[i2][j1]);
else if (ran2(seed)<prob)
    exchange(lattice[i1][j1], lattice[i2][j1]);
}

} /* End vertical bond */

} /* End Monte Carlo step */

//if past the number of MCS's to be discarded and the number of this MCS
//is a multiple of the data taking interval, take structure factor and
//correlation data, update column density histogram, and add
//instantaneous R to running sum
if ((numMCS%INTVAL==0) && (numMCS>=DISCARD))
{
    R+=Li*Lj*updatedcorr(lattice, corri, corrj,
    output)/updatedata(lattice, F, Fsq10, Fsq01, numdata);
    update_hist_data(lattice, distribution, output);
    num_avg_hist++;
}

} /* End Monte Carlo simulation */

//compute final averages for correlation functions, structure factors,
//and R
if(numdata!=0)
{
    for (int x=0; x<Ci; x++)
        corri[x]=numdata;
    for (int x=0; x<Cj; x++)
        corrj[x]=numdata;

    for (int y=0; y<Ck; y++)
        output[y]=numdata;
}


for (int i=0; i<C; i++)
    for (int j=0; j<C; j++) F[i][j]=numdata;
Fsq01/=numdata;
Fsq10/=numdata;
R/=numdata;
}
double variance01=Fsq01-F[0][1]*F[0][1];  //variance in S(0,1)
double variance10=Fsq10-F[1][0]*F[1][0];  //variance in S(1,0)

//output the results
printf(F, output);
output << "variance10=" << variance10 << endl;
output << "variance01=" << variance01 << endl << endl;
output << "R=" << R << endl;
output << "RFA=" << Li*Lj*corr[i-1][1]/F[0][1] << endl << endl;
output << "correlations in direction parallel to field" << endl;
output << "displacement" << '"' << '"' << "average correlation" << endl;
for (int x=0; x<C; x++)
    output << x << '"' << '"' << corr[x] << endl;
output << endl;
output << "correlations in direction transverse to field" << endl;
output << "displacement" << '"' << '"' << "average correlation" << endl;
for (int x=0; x<C; x++)
    output << x << '"' << '"' << corr[x] << endl;
output << endl;
printH(distribution, output, num_avg_hist);
picture(lattice, output);

return;
}

/******************************
The initialize function takes three parameters: an Li x Lj lattice array (type Grid), a char specifying the configuration to initialize to, and a pointer to the seed for the random number generator. Initialization options: r for random, v for vertical strip, h for horizontal strip, s for St. Andrew’s cross (but make certain it’s actually working correctly, i.e., preserving half-filling condition), l for L shape (but make certain it’s actually working correctly). The function traces the lattice and initializes it accordingly so that half of the spins are +1 and half of the spins are -1.
void initialize(Grid lattice, char initialtype, long *seed)
{
    //start by setting everything to 0
    for (int i=0; i<Ll; i++)
        for (int j=0; j<Lj; j++) lattice[i][j]=-1;

    //random configuration
    if (initialtype=='r')
    {
        //change -1 spins to +1 until half of spins are of each type
        for (int upspins=0; upspins<Ll*Ll/2;)
        {
            int a;
            int b;

            //choose random site on lattice
            a=int(ran2(seed)*Ll);
            b=int(ran2(seed)*Ll);

            //if site is not 1, change it to 1
            if (lattice[a][b]!=1)
                {
                    lattice[a][b]=1;
                    upspins++;
                }
        }
    }

    //horizontal strip
    else if (initialtype=='h')
    {
        int i=0;
        int j=0;
        for (int upspins=0; upspins<(Ll*Ll/2); upspins++)
        {
            if (j==Lj)
                {
                    j=0;
                    i++;
                }
            lattice[i][j]=1;
            j++;
        }
    }
}
//vertical strip
else if (initialtype=="v")
{
  int i=0;
  int j=0;
  for (int upspins=0; upspins<(Li*Lj)/2; upspins++)
  {
    if (i==Li)
    {
      i=0;
      j++;
    }
    lattice[i][j]=1;
    i++;
  }
}

else if (initialtype=="s") //Saint Andrew's cross (X shape)
{
  if (Li<=Lj)
  {
    int numup=0;

    int ic=int(float(Li)/2);
    int jc=int(float(Lj)/2);

    float slope, intercept;

    int i=0;
    int j=0;

    float a, b, area;

    for (j=0; j<=jc-2; j++)
    {
      slope=-float(Li-ic)/jc;

      a=Li+slope*j;
      b=Li+slope*(j+1);

      area = b-int(b) + 0.5*(a-b);

      int imax;
      if (int(a)>int(b) && (a-1)!=b)
imax=int(b);
else if (area>0.5)
    imax=int(b);
else imax=int(b-1);

for (i=0; i<=imax; i++)
{
    lattice[i][j]=1;
    numup++;
}
}

for (j=jc+1; j<Lj; j++)
{
    slope=\text{float}(Li-ic)/(Lj-jc);

    intercept=-slope*jc+ic;

    a=intercept+slope*j;
    b=intercept+slope*(j+1);

    area = a-int(a) + 0.5*(b-a);

    int imax;

    if (int(a)<int(b))
        imax=int(a);
    else if (area>0.5)
        imax=int(a);
    else imax=int(a-1);

    for (i=0; i<=imax; i++)
    {
        lattice[i][j]=1;
        numup++;
    }
}

for (j=0; j<=jc-2; j++)
{
    slope=\text{float}(ic)/jc;

    a=slope*j;
    b=slope*(j+1);

    area = a-int(a) + 0.5*(b-a);
int imax;

if (int(a)<int(b)&&(b-1)!=a)
    imax=int(a);
else if (area>0.5)
    imax=int(a);
else imax=int(a-1);

for (i=0; i<=imax; i++)
{
    lattice[i][j]=-1;
    numup--;
}
}

for (j=jc+1; j<Lj; j++)
{
    slope=-float(ic)/(Lj-jc);
    intercept=-slope*jc+ic;
    a=intercept+slope*j;
    b=intercept+slope*(j+1);

    area = b-int(b) + 0.5*(a-b);

    int imax;

    if (int(a)>int(b))
        imax=int(b);
    else if (area>0.5)
        imax=int(b);
    else imax=int(b-1);

    for (i=0; i<=imax; i++)
    {
        lattice[i][j]=-1;
        numup--;
    }
}

if (lattice[ic-1][jc-1]!=1)
{
    lattice[ic-1][jc-1]=1;
    numup++;
}
if (lattice[ic][jc]!=1)
{
    lattice[ic][jc]=1;
    numup++;
}
if (lattice[0][Lj-1]!=-1)
{
    lattice[0][Lj-1]=-1;
    numup--;
}
if (lattice[Li-1][0]!=-1)
{
    lattice[Li-1][0]=-1;
    numup--;
}

int difference;

difference=(Li*Lj)/2-numup;

if (difference>0)
{
    if (lattice[ic-1][jc-2]!=1)
    {
        lattice[ic-1][jc-2]=1;
        numup++;
    }
    if (lattice[ic][jc+1]!=1)
    {
        lattice[ic][jc+1]=1;
        numup++;
    }
}

difference=(Li*Lj)/2-numup;

if (difference!=0)
    cout << "error!!" << endl;

else if (Li>Lj)
{
    int numup=0;
}
int ic=int(float(Li)/2);
int jc=int(float(Lj)/2);

float slope, intercept;

int i=0;
int j=0;

float a, b, area;

for (i=0; i<=ic-2; i++)
{
    slope=-float(Lj-jc)/ic;
    a=Lj+slope*i;
    b=Lj+slope*(i+1);
    area = b-int(b) + 0.5*(a-b);

    int jmax;
    if (int(a)>int(b)&&(a-1)!=b)
        jmax=int(b);
    else if (area>0.5)
        jmax=int(b);
    else jmax=int(b-1);

    for (j=0; j<=jmax; j++)
    {
        lattice[i][j]=1;
        numup++;
    }
}

for (i=ic+1; i<Li; i++)
{
    slope=float(Lj-jc)/(Li-ic);
    intercept=-slope*ic+jc;
    a=intercept+slope*i;
    b=intercept+slope*(i+1);
    area = a-int(a) + 0.5*(b-a);

    int jmax;
if (int(a)<int(b))
  jmax=int(a);
else if (area>0.5)
  jmax=int(a);
else jmax=int(a-1);

for (j=0; j<=jmax; j++)
{
  lattice[i][j]=1;
  numup++;
}

for (i=0; i<=ic-2; i++)
{
  slope=float(jc)/ic;
  a=slope*i;
  b=slope*(i+1);
  area = a-int(a) + 0.5*(b-a);

  int jmax;
  if (int(a)<int(b)&&(b-1)!==a)
    jmax=int(a);
  else if (area>0.5)
    jmax=int(a);
  else jmax=int(a-1);

  for (j=0; j<=jmax; j++)
  {
    lattice[i][j]=-1;
    numup--;
  }
}

for (i=ic+1; i<Li; i++)
{
  slope=-float(jc)/(Li-ic);
  intercept=-slope*ic+jc;
  a=intercept+slope*i;
  b=intercept+slope*(i+1);
area = b-int(b) + 0.5*(a-b);

int jmax;

if (int(a)>int(b))
    jmax=int(b);
else if (area>0.5)
    jmax=int(b);
else jmax=int(b-1);

for (j=0; j<=jmax; j++)
{
    lattice[i][j]=-1;
    numup--;
}

if (lattice[ic-1][jc-1]!=1)
{
    lattice[ic-1][jc-1]=1;
    numup++;
}
if (lattice[ic][jc]!=1)
{
    lattice[ic][jc]=1;
    numup++;
}
if (lattice[0][Lj-1]!=-1)
{
    lattice[0][Lj-1]=-1;
    numup--;
}
if (lattice[Li-1][0]!=-1)
{
    lattice[Li-1][0]=-1;
    numup--;
}

int difference;

difference=(Li*Lj)/2-numup;

if (difference>0)
{
    if (lattice[ic-2][jc-1]!=1)
```c++
{
    lattice[ic-2][jc-1]=1;
    numup++;
}

if (lattice[ic+1][jc]!=1)
{
    lattice[ic+1][jc]=1;
    numup++;
}
}
difference=(Li*Lj)/2-numup;
if (difference!=0)
    cout << "error!!" << endl;
}
}
else if (initialtype=='1')
{
    int totup=(Li*Lj)/2;
    int numup=0;
    int numperside=int(Li*Lj*(2-sqrt(2))/2);

    int imax1;
    int jmax1;
    int imax2;
    int jmax2;

    //going along vertically
    for (int j=0; j*Li<numperside; j++)
    {
        for (int i=0; j*Li+i<numperside && i<Li; i++)
        {
            lattice[i][j]=1;
            numup++;
            imax1=i;
            jmax1=j;
        }
    }

    //going along horizontally
    for (int i=0; i*Li<numperside; i++)
    {
        for (int j=0; i*Li+j<numperside && j<Lj; j++)
        {
```
```c
{ 
    if (lattice[i][j]!=1)
    {
        lattice[i][j]=1;
        numup++;
    }
    imax2=i;
    jmax2=j;
}

if (Lj>Li)
{
    while(numup<totup)
    {
        jmax2=(jmax2+1)%Lj;
        imax2=(jmax2!=0) ? imax2 : imax2+1;

        if (lattice[imax2][jmax2]!=1)
        {
            lattice[imax2][jmax2]=1;
            numup++;
        }
    }
}
else
{
    while(numup<totup)
    {
        imax1=(imax1+1)%Li;
        jmax1=(imax1!=0) ? jmax1 : jmax1+1;

        if (lattice[imax1][jmax1]!=1)
        {
            lattice[imax1][jmax1]=1;
            numup++;
        }
    }
}
}```
{  
lattice[imax1][jmax1]=1;  
numup++;  
}

if (numup<totup)
{
  jmax2=(jmax2+1)%Lj;
  imax2=(jmax2!="0")? imax2 : imax2+1;

  if (lattice[imax2][jmax2]!=1)
    {  
lattice[imax2][jmax2]=1;  
       numup++;  
    }
}
}
}

return;
}

/**************************************************************************
The picture function takes an Li x Lj lattice array of +1’s and -1’s and an output file stream. It
prints a picture of the lattice ot the output file, representing +1 by + and -1 by 0.
**************************************************************************/

void picture(Grid lattice, ofstream& output)
{  
  for (int i=0; i<Li; i++)
    {
      for (int j=0; j<Lj; j++)
        {
          if (lattice[i][j]==1)
            output << '+';
          else output << '0';
        }
      output << endl;
    }

  /**************************************************************************

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The exchange function switches two integers that are passed by reference.

void exchange(int& a, int& b)
{
    int temp=a;
    a=b;
    b=temp;
    return;
}

float updatedata(Grid lattice, StructFact F, double& Fsq10, double& Fsq01,
                  int& numdata)
{
    // F[i][j] is structure factor for k=(i*2*PI/Li, j*2*PI/Lj)
    float F01;
    for (int i=0; i<C; i++)
    {
        for (int j=0; j<C; j++)
        {
            double kx=i*2*PI/Li; //x component of k vector
            double ky=j*2*PI/Lj; //y component of k vector
            double fRE=0.0; //real part of the Fourier transform the spin number
            double fIM=0.0; //imaginary part of the Fourier transform the
                            //spin number
            for (int x=0; x<Li; x++)
            {
                for (int y=0; y<Lj; y++)
                {
                    double kr=kx*x+ky*y; //k dot (x, y)
                    fRE+=lattice[x][y]*cos(kr);
                    fIM+=lattice[x][y]*sin(kr);
                }
            }
        }
    }
}

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```c
}
}
double f=(fRE*fRE+fIM*fIM)/Li/Lj; //instantaneous structure factor
F[i][j]+=f; //add instantaneous structure factor to running sum

//add instantaneous values to running sums of S(0,1)^2 and S(1,0)^2
if (i==0 && j==1)
{
    F01+=f*f;
    F01=f;
}
else if (i==1 && j==0)
    F010+=f*f;
}
numdata++;
return F01;
}

/**********************
This function, updatecorr, collects correlation function data,
adding new values to running sums. It takes the following
parameters: the lattice array, the running sum of correlations
in the i direction, and the running sum of correlations in the
j direction. It returns the instantaneous G(Li/2,0).
***************************/

float updatecorr(Grid lattice, Correli corri, Correlj corrj, ofstream&
                     output)
{
    float GLi20; //correlation G(Li/2,0) ((Li+1)/2 if Li is odd)
    for (int x=0; x<Ci; x++)
    {
        int corrsum=0;
        for (int i=0; i<Li; i++)
            for (int j=0; j<Lj; j++)
                corrsum+=(lattice[i][j]*lattice[(i+x)%Li][j]);
        corri[x]+=float(corrsum)/(Li*Lj);
        if (x==Ci-1)
            GLi20=float(corrsum)/(Li*Lj);
    }

    for (int x=0; x<Cj; x++)
    {
        int corrsum=0;
```
for (int i=0; i<Ll; i++)
    for (int j=0; j<Lj; j++)
        corrsun += (lattice[i][j] * lattice[i][(j+x)%Lj]);
    corrij[x] += float(corrsun)/(Li*Lj);
}
return GLi20;
}

void printF(StructFact F, ofstream& output)
{
    output.setf(ios::fixed, ios::floatfield);
    output.setf(ios::showpoint);

    output << setprecision(5);

    for (int i=0; i<C; i++)
    {
        for (int j=0; j<C; j++)
            output << setw(10) << F[i][j];
        output << endl;
    }
    return;
}

void update_hist_data(Grid lattice, Hist distribution, ofstream& output)
{
    int count = 0;

    for (int j=0; j<Lj; j++)
    {
        for (int i=0; i<Ll; i++)
        {
            if (lattice[i][j] == 1) count++;
            if (count > maxcount) { output << count; maxcount = count; output << endl;
    }
}

}
distribution[count]++;
count = 0;
}
return;
}

/*******************************************************************************/
printH prints a (picture of) the histogram.
*******************************************************************************/

void printH(Hist distribution, ofstream& output2, double num_avg_hist)
{
    output2 << endl << endl << "Histogram # " << num_avg_hist + 1 << endl;

    for(int i=0; i<=Li; i++)
    {
        output2 << distribution[i] << endl;
    }

    output2 << endl;

    for(int i=0; i<=Li; i++)
    {
        for(int d=0; d<distribution[i]/(num_avg_hist+1)/2; d++)
            output2 << "*";
        output2 << endl;
    }

    output2 << endl << endl << endl;
    return;
}

/*******************************************************************************/
/* cleardist sets all elements of distribution to 0 */
/*******************************************************************************/

void cleardist(Hist distribution)
{
    for(int i = 0; i <= Li; i++)
        distribution[i] = 0;
    return;
}
/***************************************************************************/
This function is L’Ecuyer’s long period random number generator. It has a period of about 2.3e18. Call with idum a negative integer to initialize; thereafter, do not alter idum between successive deviates in a sequence. Returns a uniform random deviate between 0.0 and 1.0 (endpoints excluded). The C code for the function comes from Numerical Recipes in C, 2nd edition.
***************************************************************************/

#define IM1 2147483563
#define IM2 2147483399
#define AM (1.0/IM1)
#define IMM1 (IM1-1)
#define IA1 40014
#define IA2 40692
#define IQ1 53668
#define IQ2 52774
#define TR1 12211
#define TR2 3791
#define NTAB 32
#define NDIV (1+IMM1/NTAB)
#define EPS 1.2e-7
#define RNMX (1.0-EPS)

float ran2(long *idum)
{
    int j;
    long k;
    static long idum2=123456789;
    static long iy=0;
    static long iv[NTAB];
    float temp;

    if (*idum<=0)
    {
        if (*((long) idum)<1) *idum=1;
        else idum=-(long) idum;
        idum2=*idum;
        for (j=NTAB+7; j>=0; j--)
        {
            k=(long) idum/IRQ1;
            *idum=IA1*(idum-k*IRQ1)-k*TRQ1;
            if (*idum<0) *idum+=IM1;
            if (j<NTAB) iv[j]=*idum;
        }
        iy=iv[0];
    }

    if (j)<NTAB) return (idum2*am + iy)*EPS;
    else return (idum2*am + iy)*EPS;
}
\}
k=(*idum)/IQ1;
*idum=IA1*(idum-k*IQ1)-k*IR1;
if (*idum<0) *idum+=IM1;
k=idum2/IQ2;
*idum2=IA2*(idum2-k*IQ2)-k*IR2;
if (*idum2<0) *idum2+=IM2;
j=iw/WDIV;
iy=iv[j]-*idum2;
iv[j]=*idum;
if (iy<1) iy+=IMM1;
if ((temp=AM*iw)>RNMX) return RNMX;
else return temp;
\}
Vita

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