TITLE

NUMERICAL INVESTIGATIONS OF HYPERSONICAL

AND REAL SPACE RENORMALISATION GROUP

TRANSFORMATIONS IN THE THREE

DIMENSIONAL ISING MODEL

Thesis

submitted by

CHARLES EDWARD WALL

for the degree of

DOCTOR OF PHILOSOPHY

Department of Physics

University of Edinburgh

August 1986
DEDICATION

I would like to dedicate this thesis to my parents, Molly and Fred, both of whose love, wisdom and sense of humour have respectfully and consistently acted as: support; an example; and a hard act to follow.
DECLARATION

The work in this thesis is entirely my own, except where otherwise indicated. Publications are in preparation concerning: the hyperscaling test of chapter 2; the effective coupling constant flow calculated in chapter 3; the optimised Monte Carlo Renormalisation group simulation of chapter 4; and the results of the fast algorithm comparisons mentioned in chapter 5.

29th August, 1986.
ACKNOWLEDGEMENTS

I should like to thank my supervisor David Wallace for his help and encouragement during the course of my research.

I am greatly indebted to the originators, Stewart Reddaway, Kevin Smith and David Scott, for the very fast Ising configuration and random number generating code so crucial to the extensive hyperscaling investigation of chapter 2. I am particularly grateful to David Scott both for helping me with APAL code and for useful suggestions concerning the setting up of the optimised Monte Carlo renormalisation group simulation of chapter 4.

For the high quality Monte Carlo renormalisation group data, which is the basis for chapter 3, and for the code which generated it, I am very grateful to Stuart Pawley. I must also thank Raul Toral for his help in developing the fast code discussed in chapter 5 and for the test of the random number generator used in chapter 2, and Chris Harris for help with chapter 5.

In addition I should like to acknowledge the Science and Engineering Research Council studentship, International Computers Limited for developing and providing support for the Distributed Array Processors at Edinburgh, and Edinburgh Regional Computing Centre for their support in various computational aspects of this work.

Penultimately it is a great pleasure to thank all the staff and students in the Physics group at Edinburgh for the support, discussions and friendship I have enjoyed over the past three years, particularly Clive Baillie, Adam Bennett, Ken Bowler, Alasdair Brown, Catherine Chalmers, David Chalmers, Roderick Dewar, Stephen Goodyear, Marifi Guler, Simon Hands, Richard Kenway, Donald McLeod, David Nicolaides, Peter Osborne, Brian Pendleton, Duncan Roweth and Barry Tynemouth.

Finally I thank Mark Cropper, Bill Zachs and Isabelle Destor for their unique brands of friendship.
ABSTRACT

In this thesis Monte Carlo simulations are presented of the three dimensional Ising model with periodic boundary conditions on simple cubic lattices of size \( L = 2, 4, 8, 16, 32, 64, \) and 128 using the International Computers Limited (ICL) Distributed Array Processor (DAP). Firstly a finite size scaling numerical experiment is performed to test for violation of hyperscaling. State of the art fast algorithms allow lattices to be simulated with high statistics. No evidence is found for violations of hyperscaling and critical exponents are obtained with an accuracy comparable to that from all other methods. Standard Monte Carlo Renormalisation Group (MCRG) analysis is extended to estimate the flow of effective couplings, to find the position of the fixed point and to map out the critical hypersurface. The results confirm the picture of the standard fixed point and allow an improved action in the basis of measured spin operators to be found. Ideas for improving MCRG are reviewed and the optimised MCRG due to Swendsen implemented. The preliminary results for small lattices indicate that this procedure is successful in making the Ising model an apparent stationary point of the Renormalisation Group (RG) transformation as far as coupling constant flow is concerned but the enhanced convergence of exponents seen by Swendsen is not obtained. The suggestion is that with our choice of real space renormalisation group kernel we are not in fact any closer to the fixed point as measured by the eigen-perturbations in the scaling fields. It is still possible that this approach could be of numerical advantage. Finally fast Ising spin configuration for canonical, microcanonical and demon ensembles is reviewed. Various limits of Creutz' demons are implemented and compared with the canonical Metropolis algorithm in terms of both computing speed and real time to generate independent configurations. This work benchmarks the DAP as an ideal machine for simulation in parallel bit manipulation problems, where it out performs state of the art supercomputers.
<table>
<thead>
<tr>
<th>Number</th>
<th>Section Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Introduction to the Modern Theory of Critical Phenomena</td>
<td>-1-</td>
</tr>
<tr>
<td>1.1</td>
<td>Introduction to critical phenomena</td>
<td>-1-</td>
</tr>
<tr>
<td>1.2</td>
<td>Description of critical phenomena in terms of discrete spin systems</td>
<td>-6-</td>
</tr>
<tr>
<td>1.3</td>
<td>Schemes for evaluating canonical averages</td>
<td>-11-</td>
</tr>
<tr>
<td>1.4</td>
<td>Renormalisation theory for Ising like spin systems: basic strategy</td>
<td>-12-</td>
</tr>
<tr>
<td>1.5</td>
<td>RSRG for Ising spins on a hypercubic lattice</td>
<td>-14-</td>
</tr>
<tr>
<td>1.6</td>
<td>Finite size scaling</td>
<td>-24-</td>
</tr>
<tr>
<td>1.7</td>
<td>An introduction to computer studies of phase transitions</td>
<td>-30-</td>
</tr>
<tr>
<td>1.8</td>
<td>Research Projects</td>
<td>-34-</td>
</tr>
<tr>
<td>2</td>
<td>Numerical Tests for Hyperscaling Violation in the Three Dimensional Ising Model</td>
<td>-36-</td>
</tr>
<tr>
<td>2.1</td>
<td>Introduction</td>
<td>-36-</td>
</tr>
<tr>
<td>2.2</td>
<td>What is hyperscaling?</td>
<td>-37-</td>
</tr>
<tr>
<td>2.3</td>
<td>Tests of hyperscaling in MC numerical work</td>
<td>-42-</td>
</tr>
<tr>
<td>2.4</td>
<td>Computational aspects of the MC test on the ICL distributed array processor</td>
<td>-45-</td>
</tr>
<tr>
<td>2.5</td>
<td>Results</td>
<td>-60-</td>
</tr>
<tr>
<td>2.6</td>
<td>Conclusions</td>
<td>-80-</td>
</tr>
<tr>
<td>3</td>
<td>Monte Carlo Renormalisation Group and Coupling Constant Flow</td>
<td>-81-</td>
</tr>
<tr>
<td>3.1</td>
<td>Introduction</td>
<td>-81-</td>
</tr>
<tr>
<td>3.2</td>
<td>The standard simulation</td>
<td>-86-</td>
</tr>
<tr>
<td>3.3</td>
<td>Estimating the critical nearest neighbour coupling and coupling constant flow</td>
<td>-87-</td>
</tr>
<tr>
<td>3.4</td>
<td>Results for the 3 d Ising model</td>
<td>-92-</td>
</tr>
<tr>
<td>4</td>
<td>Improvements on MCRG</td>
<td>-98-</td>
</tr>
<tr>
<td>4.1</td>
<td>Introduction</td>
<td>-98-</td>
</tr>
<tr>
<td>4.2</td>
<td>Optimising the RSRG in MCRG</td>
<td>-102-</td>
</tr>
<tr>
<td>4.3</td>
<td>The OMCRG performed at Edinburgh</td>
<td>-106-</td>
</tr>
<tr>
<td>4.4</td>
<td>Preliminary results</td>
<td>-109-</td>
</tr>
<tr>
<td>5</td>
<td>Fast Ising Code</td>
<td>-122-</td>
</tr>
<tr>
<td>5.1</td>
<td>Introduction</td>
<td>-122-</td>
</tr>
<tr>
<td>5.2</td>
<td>Very fast algorithms for generating Ising spin configurations</td>
<td>-124-</td>
</tr>
</tbody>
</table>
INTRODUCTION TO THE MODERN THEORY OF CRITICAL PHENOMENA

1.1. Introduction to critical phenomena

There are many varied phenomena in nature which exhibit critical behaviour [Stanley (1971); Fisher (1983)]. The prototype example is the magnetic order-disorder phase transition observable in ferromagnetic nickel on heating up to the Curie temperature, $T_C$, in the absence of an external magnetic field. Below this temperature nickel is found to exhibit a spontaneous magnetization which disappears as $T_C$ is reached in a manner described by

$$m \sim |t|^\beta$$

where $t = (T-T_C)/T_C$ is the reduced temperature and $\beta$ a critical exponent. Above $T_C$ the spontaneous magnetization is zero. Other examples of critical behaviour include the critical opalescence observable in carbon dioxide at its critical point and the liquid-gas transition of water at its critical point.

Many systems of interest have been investigated. The system, say a ferromagnet, is probed by varying each control parameter in turn and measuring quantities of interest. From the results, a phase diagram for the system can be constructed with an axis for each control parameter. Quantities of interest have to be chosen to characterise the behaviour under scrutiny. For most regions of control parameter space the values taken by observables change smoothly with each parameter. There emerge, however, distinct phases in control parameter space. These distinct phases are typified by a non-zero order parameter which becomes zero in other distinct phases. The interfaces, or more generally hypersurfaces, in control parameter space which mark the boundaries of distinct phases of behaviour are the particular areas on to which the modern theory of phase transitions and critical phenomena endeavours to shed some light.

The modern classification of the transformations between different phases is that the transition is first order if the first derivative of the free energy is discontinuous and second order or continuous where only derivatives higher than the $1^{\text{st}}$ are discontinuous. In this way the severity of the phase transition
is classified. The phase diagram of water, which provides a simple and familiar example, consists of a line of 1st order transitions corresponding to boiling water where there is a discontinuity in the specific heat due to the latent heat of vaporisation. This line is terminated by the critical point where the liquid-gas density difference (the order parameter in this case) disappears together with the latent heat of vaporisation and the transition becomes continuous. It is with continuous phase transitions and their so called critical behaviour that this thesis is concerned.

What characterises a continuous phase transition? It turns out that the behaviour of observables close to the critical hypersurface in the space of all control variables (pressure, temperature, external magnetic field etc...) can be described mathematically in terms of simple power law behaviour. Critical exponents specify the power law to which behaviour tends asymptotically and hence indicate how sharply various quantities diverge, or fall to zero, as the relevant parameters take the system through the critical hypersurface. Further from the critical hypersurface the simple power law or scaling relation between observables and relevant control parameters (or combination) has to be extended and corrections to this scaling due to the effect of irrelevant control parameters have to be added.

Physically what characterises critical behaviour is the dramatic growth of fluctuations close to and in the critical hypersurface of control parameters. A system, which away from criticality has spatial and temporal correlations only over short space and time intervals, is seen to fluctuate on all length scales up to a distance called the correlation length, $\xi$, which is seen to diverge at criticality.

In the case of the magnetic order-disorder transition, as exhibited by nickel, the standard picture is that there are two control parameters of relevance namely the reduced temperature, $t$, and the external magnetic field, $h$. Bulk observables of interest include: the net magnetisation, the susceptibility i.e. the response of system's magnetisation to a small change in the applied magnetic field $h$, higher moments of magnetisation, the internal energy, the specific heat and higher moments of the internal energy. Correlation functions which measure how much the behaviour at spatially separated regions is correlated, are a particularly good measure of the degree of co-operation between microscopic degrees of freedom. This co-operation turns out to be the essence of the macroscopically large fluctuations typical of critical phenomena.
The asymptotic scaling forms for various quantities describing a system which exhibits critical behaviour with 2 relevant parameters (t and h here) close to and at criticality are given in table (1.1). The magnet-liquid analogy is indicated. The critical exponents for the uni-axial ferromagnet order-disorder and the liquid gas phase transitions at their respective critical points have been measured and calculated and appear to be the same [Levy, Guillou and Zinn-Justin (1980)]. The best critical exponent estimates for these two systems are given for future reference. In fact there are whole families of different systems which exhibit critical behaviour described by the same power laws, critical exponents and universal functions. Such systems are said to belong to the same universality class; uni-axial ferromagnets, liquid-vapour transitions at criticality and binary alloy mixtures all being prototype examples.
<table>
<thead>
<tr>
<th>Quantity</th>
<th>Scaling Form</th>
<th>Experimental Value</th>
<th>Theoretical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific heat</td>
<td>$t^{-\alpha}$</td>
<td>$\alpha = 0.112(5)$</td>
<td>$\alpha = 0.105(7)$</td>
</tr>
<tr>
<td>Spontaneous magnetisation</td>
<td>$t^{1/2}$</td>
<td>$\beta = 0.326(2)$</td>
<td>$\beta = 0.328(4)$</td>
</tr>
<tr>
<td>Zero field magnetic susceptibility</td>
<td>$t^{-\gamma}$</td>
<td>$\gamma = 1.236(8)$</td>
<td>$\gamma = 1.2395(4)$</td>
</tr>
<tr>
<td>Spontaneous magnetisation</td>
<td>$h^{1/\delta}$</td>
<td>$\delta = 4.78(7)$</td>
<td></td>
</tr>
<tr>
<td>4th derivatives of free energy w.r.t. external field h</td>
<td>$t^{-(\gamma + 2\Delta)}$</td>
<td>$\Delta = 1.567(4)$</td>
<td></td>
</tr>
<tr>
<td>Order parameter correlation function</td>
<td>$e^{-R/\xi}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Order parameter correlation length</td>
<td>$t^{-\nu}$</td>
<td>$\nu = 0.625(5)$</td>
<td>$\nu = 0.632(1)$</td>
</tr>
<tr>
<td>Critical order parameter correlation function</td>
<td>$1/R^{d-1+\eta}$</td>
<td></td>
<td>$\eta = 0.039(4)$</td>
</tr>
</tbody>
</table>

Table (1.1) Critical exponents for the Ising universality class; the experimental values quoted are taken from various articles in Levy, Guillou and Zinn-Justin (1980), the theoretical values from Fisher and Chen (1985).

* A priori critical exponents might be expected to differ depending on how the critical point (or hypersurface) is reached. Traditionally $\alpha'$, $\gamma'$, $\Delta'$, $\nu'$ are the critical exponents when the critical temperature is reached from below. Another aspect of the universality of critical behaviour is drawn from the experimental fact that dashed and undashed critical exponents always seem to agree whenever they are both defined.

Recognising the important features which distinguish different universality classes is by no means trivial and requires much insight. The principal ones
are the number of spatial dimensions, the internal symmetries and the number of states available to the microscopic degree of freedom, the qualitative features of the interaction of microscopic degrees of freedom such as whether it is long or short in range and the way in which control parameters, such as magnetic field and temperature, couple to the system.

In this thesis the Ising universality class, to which the uni-axial ferromagnet order-disorder and the liquid-gas critical behaviour both belong, is singled out for attention. The reasons are twofold. Firstly it provides a framework for describing with the use of the Ising model familiar critical phenomena. Secondly the simplicity of the Ising model, which is used to represent the class, offers a particularly uncluttered route to gaining insight on the critical phenomena describable by the Ising universality class.

The static scaling hypothesis of Widom (1965) reproduces all the thermodynamic scaling relations in table (1.1) by asserting that the equation of state is a generalized homogeneous function of the form

\[ M(t,h) = h^{1/\delta} W(t|h|^{-\Delta}). \]  

Widom scaling has now been understood as a consequence of the correlation length scaling hypothesis of Fisher (1967). This hypothesis says there is only one length scale in the problem, the correlation length, which is sufficient to reproduce both thermodynamic and correlation type scaling relations in table (1.1). The droplet within droplet picture [Kadanoff (1967); Bruce and Wallace (1983)] generalising from the low temperature description of Ising spin systems provides a particularly intuitive picture of the physics underlying the observation of scaling on the low temperature side of the phase transition.

The many length scales in the droplet picture of a spin system approaching criticality from below \( T_c \) also arise in the following high temperature argument. Changes (fluctuations) in thermodynamic properties of the system are transported (dissipated) via the interactions between spins, \( \sigma \), connected through \( H(\sigma) \), the Hamiltonian which gives the energy for a given configuration of spins. These interactions tend to correlate neighbouring spins connected via couplings present in \( H(\sigma) \) and so correlate regions over the length scales \( a \), the distance between nearest neighbour spins interacting through \( H(\sigma) \), to the most non-local coupling. These neighbours in turn correlate their neighbours. In this way correlations over increasingly long length scales can grow. The
existence of large regions of correlated spins becomes possible as a product of the co-operation first on the microscopic length scales in $H(a)$ then on multiples of these length scales as each neighbour interacts with its connected neighbours. At high temperatures, where the Boltzmann probability factor, $\exp(-H(a)/k_B T)$, is well approximated by a power series expansion in $1/T$, these correlation effects are weak and the correlation length small. As $T$ decreases to $T_c$, it is these correlations on all length scales which give rise to the macroscopic fluctuations characteristic of critical behaviour near the phase transition point and which issue such a challenge to theoretical description. A theory of critical phenomena is necessarily tied up with solving a complex many body problem, one for each length scale. Away from criticality correlation between spins falls off rapidly with distance and the problem decouples to a large set of few body problems.

A triumph of the modern theory of phase transitions and critical phenomena has been to provide a framework in which to understand the macroscopic phenomena of critical behaviour as consequences of microscopic properties of the system. The universal features of critical phenomena put heavy demands on a successful theory. Somehow the microscopic degrees of freedom which interact in some local manner must co-operate to produce the observed macroscopic fluctuations and in the process the details of the interactions must be washed out. The problem is a many body one and much of the progress in understanding has gone hand in hand with developing tractable ways of going from the microscopic to the macroscopic. The renormalisation group [Wilson (1971)] has provided the key framework in which to achieve this.

This thesis is primarily concerned with showing how finite size scaling (critical phenomena in finite systems) and renormalisation group methods can be used in conjunction with a powerful parallel computer to elucidate critical behaviour in the Ising model.

1.2. Description of critical phenomena in terms of discrete spin systems

The Ising model [Ising (1925)] is a particularly elegant and simple model which can be regarded as describing the essential microscopic features of systems as diverse as a uni-axial magnetic crystal a lattice gas or an uni-axial ferroelectric. The exact solution of the one dimensional [Ising (1925)] and the two dimensional [Onsager(1944)] pure spin one half Ising models have provided invaluable theoretical anchor points with which to compare other
models and also form a stringent benchmark against which to test approximation schemes proposed for analysing more complicated systems. As such the various observables are expected to scale asymptotically as in table (1.1). The three dimensional pure spin one half Ising model on a finite lattice is expected to exhibit the finite pre-cursors, the so called pseudo-critical behaviour, of bulk critical behaviour. The theory of finite size scaling indicates that the various finite observables should scale as in table (1.1) as L becomes infinite, and in a way determined by the bulk critical exponents for finite L. As such the various observables are also expected to scale asymptotically as in table (1.1). The model has been subjected to many approximate schemes though no exact solution has been found. The simplicity of the model lends itself to computer simulation and as such represents the easiest computational route to the critical behaviour of the Ising universality class. In view of the above the pure spin one half Ising model in three spatial dimensions constitutes an excellent testing ground for computational schemes which might yield new information on an unsolved problem.

Consider a d dimensional hypercubic lattice of linear spatial extent, L in units of lattice spacing, a. At each site, i, on the lattice an Ising spin, σ_i, exists which can take values from the set {+1,-1} corresponding to the spin pointing "up" or "down" in the easy direction. The interaction energy of the system of L^d Ising spins is given by

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$  \hspace{1cm} (1.3)

where \(\sum_{\langle i,j \rangle}\) indicates that the sum is to be performed over all nearest neighbour pairs of Ising spins on the lattice. \(H(\sigma)\) acts as a reminder that the Hamiltonian depends on the pattern or configuration, \(\sigma\), formed by the \(L^d\) Ising spins. The interaction constant \(J>0\) corresponds to a ferromagnetic system where the individual spins prefer to be aligned. The case \(J<0\) corresponds to an antiferromagnet where nearest neighbouring spins prefer to be oppositely aligned. With periodic boundary conditions the Hamiltonian, equation (1.3), is homogeneous and translationally invariant. Note also the overall/global up-down symmetry.
The addition of an uniform external magnetic field, \( h \), which couples to each \( \sigma_i \), breaks this "up-down" symmetry and the Hamiltonian becomes

\[
H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i. \tag{1.5}
\]

the Ising model in an uniform external field, where \( \sum \) is over all spins on the lattice.

A macroscopic statistical average for a quantity \( A \) is indicated by \( \langle A \rangle \) and is obtained as a thermodynamic average over the ensemble of possible microstates or spin configurations denoted by

\[
\{ \sigma \} = \{ \sigma_1 = \pm 1, \sigma_2 = \pm 1, \ldots, \sigma_N = \pm 1 \} \tag{1.6}
\]

Such canonical averages are written

\[
\langle A \rangle = \sum_{\{ \sigma \}} A(\sigma) P(\sigma) \tag{1.7}
\]

where \( P(\sigma) \) is the probability of configuration \( \sigma \) and is normalised so that

\[
\sum_{\{ \sigma \}} P(\sigma) = 1. \tag{1.8}
\]

For equilibrium statistical mechanics \( P(\sigma) \) is given by the Boltzmann distribution

\[
P(\sigma) = \exp(-H(\sigma)/k_b T)/Z \tag{1.9}
\]

where

\[
Z = \sum_{\{ \sigma \}} \exp(-H(\sigma)/k_b T); \tag{1.10}
\]

\( k_b \) is Boltzmann's constant, \( T \) is the absolute temperature and \( Z \) is the partition function.
For convenience $-1/k_bT$ will be absorbed into $H(\sigma)$ so that (1.3) can be rewritten as

$$H(\sigma) = K_{nn}S_{nn} \tag{1.11}$$

with $K_{nn} = J/k_bT$ and $S_{nn} = \sum \sigma_i \sigma_j$. Similarly equation (1.5) becomes

$$H(\sigma) = K_{nn}S_{nn} + K_hS_h \tag{1.12}$$

with $K_h = h/k_bT$ and $S_h = \sum \sigma_i$, where $K_{nn}$ and $K_h$ are called the nearest neighbour and magnetic coupling constants respectively and are dimensionless. The class of all Ising spin Hamiltonians can now be written as

$$H(\sigma) = \sum K_\alpha S_\alpha \tag{1.13}$$

where the even $S_\alpha$ are the various two, four, six... spin combinations and the odd $S_\alpha$ are one, three, five,... spin combinations. The sum over $\alpha$ in general includes all topologically distinct spin combinations that can be embedded in the lattice. The $K_\alpha$ are the respective coupling constants. The vector shorthand $H(\sigma) = KS$ is used interchangeably with the notation in (1.13) henceforth.

It is hoped the Ising model in an external field can mimic the essential features of uni-axial ferromagnetic critical phenomena. If this is so then the following observables, in the limit $L \to \infty$, should scale with $t$ and $h$ as in table (1.1), and hence offer a description of the critical phenomena exhibited by the Ising universality class. The dependence of the quantities that follow on the boundary conditions and finite size of the system are suppressed from view but not from mind.

The magnetisation per spin of the Ising model in an external field is given by

$$m(t,h) = L^{-d} <S_h> \tag{1.14}$$

where $d$ is the spatial dimension. The magnetic susceptibility per spin is an example of a response function and measures the change in magnetisation induced by a change in the externally applied magnetic field:
\[ \chi(t,h) = \frac{\partial \mu(t,h)}{\partial h}. \]  

Formally taking the derivative in equation (1.14) yields for the spin system

\[ \chi(t,h) = L^{-d} \left( k_b T \right)^{-1} \{ <S_h^2> - <S_h>^2 \}. \]  

Higher moments of magnetisation per spin are of interest and are obtained by differentiating the free energy per spin further times by \( h \) to obtain in general

\[ \frac{\partial^n f}{\partial h^n} = L^{-d} \left( k_b T \right)^{-(n-1)} <S_{h^n}>_c \]  

where \( <S_{h^n}>_c \) indicates the \( n \)th cumulant or connected moment and is obtained by subtracting the disconnected pieces from \( <S_{h^n}> \).

In the model with only nearest neighbour interactions, the specific heat per spin is given by

\[ C_h(t,h) = \frac{\partial u(t,h)}{\partial T_h} = L^{-d} \left( k_b T \right)^{-1} \left( <S_{nn}^2> - <S_{nn}>^2 \right) \]  

Correlations between spatially separate spins can be measured and are found to become large as the system approaches the phase transition i.e. as the system becomes critical. The spin-spin correlation function or two point function is defined by:

\[ G(r_i-r_j) = \langle (\sigma_i - <\sigma_i>)(\sigma_j - <\sigma_j>) \rangle. \]  

For a homogeneous system

\[ \sum_{i,j} G(r_i-r_j) = \chi(t,h)L^d \]  

which highlights the intimate way in which correlation and thermodynamic functions are related.

There are many other quantities which can be measured in order to capture the subtleties of a system at criticality; only some of the basic quantities have
been spelled out above.

1.3. Schemes for evaluating canonical averages

The calculation of various canonical averages corresponding to observables of interest is crucial if the macroscopic implications of a model are to be obtained. It is through comparing such averages with experiment that the suitability of a model to describe the physics of interest can be assessed. The behaviour of observables $<A>$ as $T$ and $h$ are varied is obtained by evaluating equation (1.7). For small systems and discrete spins each term can be evaluated and the sum over configurations calculated explicitly. The number of configurations in equation (1.7), $2^N$, grows exponentially with increasing lattice size and quickly this straightforward approach becomes impracticable. Computers can be used to enumerate exactly equation (1.7) for systems of $N \sim 30$ Ising spins. To mimic physical phenomena with $N \sim 10^{23}$ larger systems are required and ingenuity has to be used to obtain an estimate of equation (1.7) whether it be via analytic or numerical methods, with or without the use of a computer.

There are relatively few models which have been solved exactly. With the exception of the spherical model, one is restricted to one and two dimensions, in the latter case typically with zero external field and only simple (e.g. nearest neighbour) interactions. Such solutions offer some theoretical insight into how macroscopic effects are produced from microscopic rules of interaction and also provide a very stringent bench mark against which to test new schemes, but offer little insight into universality. In general (1.7) must be evaluated by some approximation scheme. Each approximation scheme has its associated systematic error which can only be estimated within the scheme. It is from the comparison of different approximation schemes offering different vantage points for insight that confidence in estimates for $<A>$ is obtained.

Of the analytic approximations used to date, e.g. series expansions and mean field methods, most involve truncation of a perturbation expansion for which the effect of neglecting an infinite number of small terms is difficult to assess. Numerical approximations schemes based on perturbation series can evaluate more terms in the series and hopefully lessen the uncontrolled truncation error. In computer simulation $<A>$ is estimated in some non-perturbative way. The uncontrolled truncation is replaced by statistical error and systematic errors due to the finite size of the system and one hopes not imperfection of
pseudo-random numbers.

The large fluctuations in $<A>$ when evaluated at or near a phase transition point together with the fluctuations on all length scales usually means in approximations such as the low temperature series or high temperature series that successive terms become of equal importance so that extrapolation techniques are required to obtain critical behaviour. In MC simulations where $<A>$ is again evaluated in one calculation on all length scales, the problems of critical slowing down and increased relaxation times and correlation distances make simulations at criticality prohibitively expensive.

The way out of the dilemma for approximate evaluation of $<A>$ at and near $T_c$ is not to attempt to evaluate $<A>$ in one (very big) calculation on all the fluctuating length scales. Instead attention is better focussed on one length scale at a time. The next section describes how the RG enables this to be realised.

1.4. Renormalisation theory for Ising like spin systems: basic strategy

There have been many advances in the understanding of critical phenomena recently due largely to the advent of renormalisation group ideas and their application to statistical mechanics problems [Wilson (1971)]. There are many good and detailed reviews of renormalisation group: see for example Wilson (1971); Wilson (1975); Wilson and Kogut (1974); Fisher (1976); Kadanoff (1978); Wegner (1976) and Wallace and Zia (1978). Here the basic strategy and its implications for Ising like spin systems is reviewed.

In tackling the problem of a system at criticality fluctuating on all length scales, a renormalisation group (RG) approach adopts the strategy of divide and conquer. Rather than evaluate equation (1.7) completely, integrating over all length scales $a$ to $L_a$ in one (very large) calculation, the RG approach seeks to integrate out fluctuations on successively longer and longer length scales. Starting with $L^d$ sites on a simple hypercubic lattice, say, and an interaction Hamiltonian $H(G) = K^0 S^0(a^0)$ with lattice spacing $a$, the first application of R removes fluctuations of length scales $a$ to $ba$ where $b$ is some scale factor greater than 1. The renormalised system contains $(L/b)^d$ first level of R block-spins $\{\sigma^1\}$ on a lattice of spacing $a' = ba$ and new effective Hamiltonian (first level of R Hamiltonian $H^1$) $H^1(\sigma^1) = K^1 S^1(\sigma^1)$. Usually the block-spins are defined to take their values from the same set as the zeroth level spins i.e. $\{+1,-1\}$ and live on a lattice of $b^d$ fewer sites and shortest length scale $b a$. 
This property of isomorphism built into $R$ allows iteration of this renormalising or pruning procedure. The details of behaviour over length scales $a$ to $b$ are lost but their long distance implications are absorbed into the coupling constants of the renormalised Hamiltonian. Each repetition of this procedure successively prunes out from the original problem a length scale, e.g. $ab^{n-1}$ to $ab^n$ on the $n^{th}$ application, and accounts for this liberty by adjusting the $K^n$ appropriately. The philosophy is that each pruning only involves a finite trace over blocks of $b^d$ spins to produce a renormalised block-spin and hence is quite tractable provided the rule for determining the block-spin is sufficiently local, and that with enough iterations the remaining problem will involve a few blocked spins interacting through a renormalised Hamiltonian whose couplings embody the universal features of the original problem. The problem of solving a many body problem interacting on all length scales is thus transformed into many small problems one for each length scale (for a discrete lattice) and a residual renormalised few body problem which is hopefully tractable.

The general implementation of the RG program can take many forms. The Hamiltonian can be itself transformed from discrete valued spins to continuous fields (e.g. Ising model to Ginsburg–Landau field theory via Hubbard–Stratonovich transformation), and it can be defined in continuous space, and tackled typically by momentum space methods.

Momentum space RG methods are discussed in Amit(1978) and essentially involve successively integrating over the upper fraction of the wave vectors of the degrees of freedom left in the problem using field theory techniques. In the real space renormalisation group (RSRG) approach the partial integration of each length scale is evaluated by some exact or approximate scheme on variables defined in real space. Examples will be described in detail in this thesis.

Having chosen a model and a renormalisation transformation analytical or numerical methods are used on each of the different length scale problems to implement the partial integration. The residual problem remaining after the blocking to length scales of the order of the correlation length is also amenable to standard approximations. The hope is that these approximate methods are more controllable in this situation where successive integrations involve systems further from criticality, than when stretched to take care of all length scales at once: the partial configuration sum at any one blocking should not be itself critical. The task of combining all the length scales again is
looked after by the renormalisation transformation.

1.5. RSRG for Ising spins on an hypercubic lattice

Since the idea of real space renormalisation was first introduced [Kadanoff (1967)] this physically intuitive method has been applied with great success to many problems [for a review see Niemeijer and van Leeuwen (1976) or Burkhardt and van Leeuwen (1982)].

In general a real space renormalisation group (RSRG) transformation $R$ can be defined via

$$\exp(G(K) + H'(c')) = \sum_{\{c'\}} P(a',a) \exp(H(c)).$$

The weight function, $P(a',a)$, specifies the rule for projecting site spins, $a_i$, on the site lattice $i = 1, ..., N$, into blocked spins, $a'_i$, on a blocked lattice, $i' = 1, ..., N'$. The block-spins or renormalised spins or cell spins, $\{a'_i\} \in \{+1,-1\}$, reside on a lattice usually chosen to be isomorphic to the original or previous RG level lattice but of spacing $a' = ba$ and spatial extent $L' = L/b$ in terms of the new lattice spacing.

The result of the weighted (or partial) sum over configurations on the r.h.s. of equation (1.21) is to produce a renormalised Hamiltonian plus an integration constant on the l.h.s. The renormalised Hamiltonian specifies how the block-spins interact and has a form $H'(\sigma) = \sum_{\sigma} K'_{\alpha} S'_{\alpha}(\sigma')$ and the set $K'$ is determined from the set $K$ in such a way as to account for the degrees of freedom that have been removed by the renormalisation transformation. $G(K)$ is independent of $\sigma'$ and constitutes the contributions to the free energy made by the short wavelength fluctuations among the $\sigma_i$ which have been integrated out of the problem.

**Conditions imposed on the weight function**

It is desirable that a real initial Hamiltonian be renormalised to a real renormalised Hamiltonian. To ensure that $G(K)$ and $H'(\sigma')$ are real, the condition,
\[ P(a',c) > 0 \quad (1.22) \]

for all \( a', a \), is sufficient but not necessary. The sufficient but not necessary condition

\[ \sum_{\{\sigma'\}} P(\sigma',\sigma) = 1 \quad (1.23) \]

can be seen, on inserting into the equation for the block-spin partition function

\[ Z' = \sum_{\{\sigma'\}} \exp(G(K) + H'(\sigma')), \quad (1.24) \]

to ensure that

\[ Z' = Z \quad (1.25) \]

and hence that the block-spin system describes the same physics as the site system. Equation (1.25) constitutes the renormalisation imposed on the couplings \( K' \).

If we require \( H'(\sigma') \) and \( H(\sigma) \) to have the same global up-down symmetry then \( P(\sigma',\sigma) \) should be chosen so as to be invariant under the simultaneous transformations \( \sigma \to -\sigma; \sigma' \to -\sigma' \) i.e.

\[ P(\sigma',\sigma) = P(-\sigma',-\sigma). \quad (1.26) \]

Within the constraints (1.22) and (1.23) there remains a lot of freedom in the choice of the weight function. In particular, the idea that the block-spin \( \sigma'_i \) should represent the effect of a local cluster of the original site spins is typically implemented by choosing a weight function which factorises as a product of terms one for each \( \sigma'_i \). More subtly, it is essential for the success of the whole method that although the full configuration sum (1.9) may be at criticality, the weighted configuration sum (1.21) is not; this feature ensures that the coupling constants \( K' \) and \( G \) should be regular functions of the coupling constants \( K \), and that \( H' \) should be short range.

For now some implications of "well behaved" weight functions will be
The free energy under renormalisation

The free energy of the original system is given by

\[ F(K) = \ln(Z). \]  \hfill (1.27)

Using equation (1.25) and substituting for \( Z' \) from (1.24) gives

\[ F(K) = G(K) + \ln\left(\sum_{\{\sigma'\}} \exp(H'(\sigma'))\right). \]  \hfill (1.28)

Identifying

\[ F'(K') = \ln\left(\sum_{\{\sigma'\}} \exp(H'(\sigma'))\right) \]  \hfill (1.29)

as nothing but the free energy of a system of block-spins interacting with
Hamiltonian, \( H'(\sigma') = K'.S'(\sigma') \), yields the following relationship between the free energy before and after the (pruning phase of the) renormalisation transformation

\[ F(K) = G(K) + F'(K'). \]  \hfill (1.30)

In the thermodynamic limit where, \( N \) the number of Ising spins, becomes very large then the free energy per degree of freedom, \( f \), should tend to some limit as is observed in experiment:

\[ F(K) = Nf(K). \]  \hfill (1.31)

Similarly,

\[ F'(K') = N'f(K'). \]  \hfill (1.32)

where \( f \) is the free energy per degree of freedom for the block-spin system.
The integration constant $G$ is a function of the unrenormalised couplings $K$ and it is expected to be as extensive as $F(K)$ so that

$$G(K) = N g(K)$$  \hspace{1cm} (1.33)

where $g$ is the integration constant per degree of freedom.

The result of the renormalisation transformation defined via, (1.21) to (1.25), on the free energy per degree of freedom is, collecting equations (1.30) to (1.33)

$$f(K) = g(K) + b^d f(K')$$  \hspace{1cm} (1.34)

with $b^d = N/N'$ the real space renormalisation scaling factor. Equation (1.34) constitutes a recurrence relation, iteration of which allows non-universal quantities to be expressed in terms of a sum of integration constants (one $g(K)$ for each length scale removed) and a residual problem on a system far from criticality (if the original system was close but not precisely at criticality). The universal features such as the critical exponents and the universal scaling function reside in the coupling constant flow.

**Realspace renormalisation as flow in coupling constant space**

After $n$ blockings the action of $R$ is to transform $H^n(K^n)$ into $H^{n+1}(K^{n+1})$ and to produce an integration constant which contributes to the free energy according to (1.34). The sequence $H^n(K^n)$ can be described by a flow in the space of all Ising Hamiltonians which can be conveniently parameterised as a flow in the space of all couplings

$$K^{n+1} = K^{n+1}(K^n)$$  \hspace{1cm} (1.35)

with $K^n = (K_1^n, K_2^n, K_3^n, \ldots)$ a vector whose components are a complete set of couplings that fit on the lattice.

With equations (1.34) and (1.35) the strategy of renormalisation theory, as far as thermodynamic quantities (near the phase transition point) are concerned, can be restated as obtaining (the singularities of) the free energy per degree
of freedom $f(K)$ (whose singularities are the pre-cursors of the divergences typical of critical behaviour which appear when a suitable number of derivatives of the $f(K)$ are taken to give the various thermodynamic quantities) from the regular (hopefully) functions $g(K)$ and $K'(K)$. There is no guarantee, a priori, that $g(K)$ and $K'(K)$ will be regular in the region of coupling constant (control parameter) space of interest; as indicated earlier, part of the renormalisation strategy is to chose $P(\sigma',\sigma)$ so that $g(K)$ and $K'(K)$ are indeed regular in the required region.

**Critical phenomena via the fixed points of a RSRG transformation**

The recursion relation (1.35) is of particular interest in the vicinity of fixed points, $K^*$ for which $K'(K^*) = K^*$. Since in an RSRG transformation, the correlation length $\xi$ in units of the lattice spacing changes by a factor $1/b$, fixed points must correspond to $\xi = 0$ or $\xi = \infty$. At critical fixed points ($\xi = \infty$) the system is scale invariant because it has the same effective interactions on all length scales. Not all fixed points represent critical points. For example $K^* = 0$ and $K^* = \infty$ are trivial fixed points corresponding to $T = \infty$ and $T = 0$ respectively for Ising systems. Corresponding to the many Ising systems in the Ising universality class, characterised by a set of non-trivial critical exponents (see table (1.1)), equation (1.34) is expected to have one non-trivial fixed point $K^*$. Where there is more than one fixed point the problem is how to distinguish fixed points of different physical interest from one another and from those which may be artefacts of the RSRG transformation and the approximation scheme.

**Linearising the Recurrence Relation**

Assuming the existence of a non-trivial fixed point $K^*$ and the analyticity of the equations, $K' = K'(K)$, then a Taylor series expansion about $K^*$ should be valid for $K'$ giving:

$$K'(K^* + (K - K^*)) = K'(K^*) + \partial K'/\partial K|_{K^*}(K - K^*) +$$
Assuming that \( O((K-K')^2) \) can be neglected for \( K \) close to \( K' \) one obtains a set of simultaneous linear equations

\[
(K'-K')_\alpha = \sum_\beta T_{\alpha \beta} (K'-K')_\beta
\]  

(1.37)

where

\[
T_{\alpha \beta} = \frac{\partial K'_\alpha}{\partial K'_{\beta}}. \tag{1.38}
\]

The matrix \( T^* \) is not symmetric a priori and so the characteristic equation

\[
|T-\lambda I| = 0
\]

which gives the eigenvalues \( \lambda_i \) associated with the normal modes, or scaling fields of the linearised renormalisation transformation induced recursion relation, equation (1.38), are not necessarily real.

**The normal co-ordinates or scaling fields of the linearised recursion relation**

Normal co-ordinates can be constructed from the eigenvectors and associated eigenvalues via the eigenvalue equation

\[
\sum_\alpha \phi^i_\alpha T^*_{\alpha \beta} = \lambda_i \phi^i_\beta
\]  

(1.39)

In matrix notation (1.39) becomes,

\[
\phi^i T^* = \lambda_i \phi^i
\]  

(1.40)

for \( \phi^i \) left eigenvectors and
\[ T^* \psi^i = \lambda_i \psi^i \quad (1.41) \]

for \( \psi^i \) right eigenvectors corresponding to the same eigenvalue \( \lambda_i \).

With the coupling constant flow linearised about the fixed point \( K^* \), the normal co-ordinate perturbations should be some linear combination of coupling constant perturbations \((K-K^*)_\alpha\).

\[ u_i = \sum_{\alpha} \phi^i_\alpha (K-K^*_\alpha) \quad (1.42) \]

with \( \phi^i_\alpha \) the amount of \((K-K^*)_\alpha\) required in the \( u_i^{\text{th}} \) scaling co-ordinate. With the choice (1.42) of normal co-ordinates the recursion relation (1.37) is diagonalised as

\[ u_i' = \lambda_i u_i. \quad (1.43) \]

In order to appreciate the implications of these equations, imagine a zeroth level Hamiltonian close to \( K^* \) such that \( u \) is small. For \( u_i \) corresponding to \( \lambda_i > 1 \) the tendency is for \( u_i < u_i^{\text{th}} < \ldots u_i^n \) on successive application of the chosen renormalisation transformation, \( R \), and the renormalised systems so generated to flow away from \( H^* \) which represents a system at \( K^* \) or \( u^* = 0 \). Such \( \lambda_i > 1 \) are called relevant eigenvalues because associated eigenperturbations become more and more significant. The corresponding eigenvectors are called relevant eigenvectors, similarly the corresponding normal co-ordinates are called relevant scaling fields. For \( \lambda_i < 1 \) the tendency on application of the chosen renormalisation transformation, \( R \), is for the corresponding irrelevant scaling fields to decrease and for the system to approach \( K^* \) in these directions. Marginal eigenperturbations are associated with eigenvalues \( \lambda_i = 1 \) and are unchanged under application of \( R \); in this case further orders in \( K-K^* \) must be retained in order to describe the flow.

Extensions beyond the linear regime also allow the description of Hamiltonian flow further from the fixed point. Such corrections to leading order give rise to, non-linear scaling fields involving in general curvilinear co-ordinates. Corrections to leading order scaling relations can be calculated from such extensions. For a full discussion see Niemeijer and Leeuwen (1976).
Free energy under renormalisation in terms of scaling fields

The equation (1.34) can now be expressed in terms of the scaling fields \( u_i(K) \) to give

\[
f(u) = g(u) + b^{-d}f(\lambda u) \tag{1.44}
\]

(Of course \( f \) and \( g \) have different functional forms for scaling fields than they had for coupling constants.) The basic assumptions of the renormalisation group approach are likewise translated. The regularity of the recursion relation \( K'(K) \) becomes the assertion that \( u(K) \) must be a regular function of \( K \) and that the eigenvalues \( \lambda \) be finite. The regularity of \( g(K) \) becomes the regularity of \( g(u) \) near the fixed point at \( u=0 \). The behaviour close to this fixed point is elegantly described by the simple scaling law (1.43) with \( \lambda_i > 1 \) relevant, \( \lambda_i < 1 \) irrelevant and \( \lambda_i = 1 \) marginal.

The following picture of universality near a "standard" fixed point arises. For a system which requires \( n \) scaling fields for its complete description of which the first \( m < n \) are relevant and the remaining \( n-m \) irrelevant (assuming there are no marginal scaling fields) there exists an attractive domain or hypersurface defined by \( u_1, u_2, \ldots, u_m = 0 \). With all the relevant perturbations set to zero iteration of equation (1.43) shows that for \( i = m+1, \ldots, n \), \( u_i \) approaches a limiting value zero, as the number of applications \( r \) of \( R \) becomes large. This corresponds to the system's arrival at the fixed point which resides in the hypersurface of irrelevant scaling fields. The universality of many different systems with their relevant scaling fields tuned to zero emerges as a result of them all residing in the critical hypersurface of attraction of the same fixed point.

The connection between the eigenvalues describing how the scaling fields change under the application of the renormalisation transformation (1.21) and the critical exponents is now indicated from the hypothesis that the free energy is dominated by a singular part of simple power form in the relevant scaling fields. This is Widom's static scaling hypothesis (1965). The RSRG calculation of the free energy \( f(u) \) in terms of the regular function \( g(u) \) (see Niemeijer (1976)) confirms that indeed the form of the free energy satisfying equation (1.44) is
\[ f(u_1,u_2,u_3\ldots) = f_{\text{reg}}(u_1,u_2,u_3\ldots) + f_{\text{sing}}(u_1,u_2,u_3\ldots) \quad (1.45) \]

and that the singular part has the homogeneity property

\[ f_{\text{sing}}(u_1,u_2,u_3\ldots) = b^{-d} f_{\text{sing}}(\lambda_1 u_1, \lambda_2 u_2\ldots) \quad (1.46) \]

which on iterating \( I \) times gives

\[ f_{\text{sing}}(u_1,u_2\ldots) = b^{-Id} f_{\text{sing}}(\lambda_1^I u_1, \lambda_2^I u_2\ldots). \quad (1.47) \]

Choosing the iteration number \( I \) such that \( \lambda_1^I |u_1| = 1 \), say, this RSRG justification for Widom scaling shows that \( f_{\text{sing}} \) has the scaling form

\[ f_{\text{sing}}(u_1,u_2\ldots) = |u_1|^{\nu_1} b^{\gamma_1} A_1^{\pm}(u_2/|u_1|^{\nu_2}, u_3/|u_1|^{\nu_3}, \ldots) \quad (1.48) \]

where

\[ b^{\gamma_1} = \lambda_1 \quad (1.49) \]

and \( u_1 \) has been singled out as the relevant scaling field of interest though any relevant field could equally well have been singled out. \( A_1^{\pm} \) expresses the fact that the corrections to leading order behaviour for \( u_1 > 0 \) and \( u_1 < 0 \) may differ.

Physically, the fixed point for critical behaviour in the Ising universality class should have only two relevant perturbations corresponding to the control parameters reduced temperature \( t \) and external field \( h \). By symmetry under spin reversal, the stability matrix \( T_{\alpha\beta} \) will factorise into sub-spaces corresponding to even and odd powers of spins and the linear scaling fields \( u_1, u_2 \) will correspond to \( t \) and \( h \).

Irrelevant perturbations have \( \lambda_i < 1 \) and hence by (1.49) \( \nu_i < 0 \). Therefore according to (1.48) as the relevant parameters such as \( u_1 \) and \( u_2 \), are tuned to zero, the effect of the irrelevant perturbations indeed become vanishingly small; they represent corrections to the leading scaling behaviour. The above discussion has been restricted to scaling in the free energy. A similar discussion of scaling of correlation functions is given in Niemeijer and van
Leeuwen (1976), where further analysis of the free energy formalism can also be found.

With the identifications, \( u_1 = t \); \( u_2 = h \), the scaling of thermodynamic quantities is obtained by taking various derivatives of the singular part of the free energy; the critical exponents are then obtained in terms of the \( \gamma_i \). For example the singular part of the magnetisation per site is given by:

\[
m(t,h,u_3) = -\partial f_{\text{sing}}(t,h,u_3)/\partial h.
\]  

(1.50)

Hence from (1.48)

\[
m(t,h,u_3) = |t|^{(d-\gamma_1)/\gamma_1} \partial A_1 \pm (h|t|^{\gamma_1}/(\gamma_1 u_3)|t|^{\gamma_2}/\gamma_2)/\partial (h|t|^{\gamma_1}/(\gamma_1 t))
\]  

which to match the definition, \( m(t) \sim |t|^\Delta \) in the limit \( t \to 0^- \) with \( h = 0 \), implies the identity requires

\[
\beta = (d-\gamma_h)/\gamma_t.
\]  

(1.52)

Taking the derivatives with respect to \( h \) of (1.51) and choosing \( \lambda \) so that \( b^{(v_h)}|h = 1 \) and then setting \( t=0 \) and \( h \to 0 \) implies with the definition \( m(t,h) \sim h^{1/\delta} \).

\[
\delta = (d-\gamma_h)/\gamma_h.
\]  

(1.53)

A further derivative with respect to \( h \) gives the susceptibility and implies the identification

\[
\gamma = (d-2\gamma_h)/\gamma_t
\]

The specific heat per spin is given by \( \partial^2 f/\partial t^2 \) and gives:

\[
\alpha = (d-2\gamma_t)/\gamma_t
\]  

(1.54)

Finally at \( h = 0, t \to 0 \), the scaling relation for the correlation length in lattice units, \( \xi' = \xi/b \), implies
So we see that the two relevant R. G. exponents $\gamma_t$ and $\gamma_h$ determine $\alpha$, $\beta$, $\gamma$, $\delta$, $\Delta$ and $\eta$ and $\nu$. The various inequality relations amongst these exponents [see Stanley (1971) or Fisher (1983)] have become equalities. Moreover not only the so-called ordinary relations amongst scaling exponents

\[ \alpha + 2\beta + \gamma = 2; \Delta = \beta \delta = \beta + \gamma; \gamma = (2 - \eta) / \nu \]  

satisfied by all soluble models to date, but also the so-called hyperscaling relations relating thermal and correlation exponents and including $d$ the dimensionality:

\[ d \nu = 2 - \alpha; \; d(\delta - 1)/(\delta + 1) = 2 - \eta; \; d \nu = 2 \Delta - \gamma, \]  

automatically arise within the RG formalism.

1.6. Finite size scaling

The critical phenomena observed in nature are macroscopic events typically involving $\sim 10^{23}$ degrees of freedom. To what extent can an Ising model with $L^d$ spins emulate such critical behaviour? A thorough understanding of the relationship between the finite estimates of bulk quantities and the bulk quantities themselves can perhaps turn finite size effects into a positive advantage by allowing useful investigations to be made with conveniently small systems and the results finite size corrected or scaled up to give the estimated bulk values of the quantities of interest. Finite size scaling [Fisher (1971); Barber (1983)] affords a basis for doing just this. In this section we discuss the finite size scaling analysis appropriate to the 3 d Ising model which for finite $L$ exhibits pseudo-critical behaviour.

Firstly consider the free energy of a system of finite extent $L$ in each dimension and $L^d$ degrees of freedom say spins away from $T_c$. For a homogeneous system and a specified interaction the expected dependence of the free energy is
where \( \tau \) is to remind us of the potential dependence on the applied boundary conditions. In the thermodynamic limit physically it is expected that the free energy per degree of freedom or per unit volume should tend to a limiting value dependent on the temperature of the system and the density of spins

\[
F^\tau = F^\tau(T,V,N)
\]

It is expected that a large but finite system will tend to this bulk limit in the following way,

\[
F^\tau(T,V,N) = \lim_{V \to \infty} \lim_{\rho \to \infty} f^\tau(\rho) = f^\tau(T,V,N)/V
\]

for \( V \) large and \( \rho \) and \( T \) fixed. The finite size correction \( O^\tau(V) \) is boundary condition dependent and is less extensive than \( V \), so that

\[
\lim_{V \to \infty} O^\tau(V)/V = 0
\]

Although the geometry of the system can be important, in this thesis the main concern is with systems of finite extent in all spatial directions and with periodic boundary conditions preserving the translational invariance and removing surface effects. Periodic boundary conditions are denoted by \( \tau = 0 \), and away from \( T_c \) have very small finite size effects:

\[
F^0(T,V,N) = Vf^0(T,\rho) + O(\exp(-L\Gamma(T)))
\]

with \( V \to \infty \) and \( T \) and \( \rho \) fixed. Near \( T_c \), \( \Gamma \) becomes very small and the finite size effects become power like.

In finite systems the apparent (pseudo) critical point is found to be shifted with respect to the critical point of the bulk system. This shift approaches the bulk \( T_c \) in a power like manner as:
with $\lambda$ the shift exponent. The position of the maximum value of the finite system’s specific heat or susceptibility versus temperature curves provides a useful definition of $T_m(L)$ for various values of $L$. Another important point on a finite size curve is $T^*(L)$ where the finite curve departs significantly from the infinite curve. The rounding temperature at which this occurs has an associated rounding exponent defined as:

$$|T^*(L) - T_c|/T_c \sim b/L^\theta$$

(1.64)

where $T^*(L)$ is the value of $T(L)$ at which, say

$$\frac{(C_\infty(T(L)) - C(T(L)))/C_\infty(T(L))}{(1.65)}$$

A successful theory of finite size scaling should allow $\lambda$ and $\theta$ to be predicted. Fisher’s finite size scaling hypothesis (1969) does just this. The key assertion leading to this hypothesis is that for a finite system temperature $T$ close to the bulk critical temperature $T_c$, the ratio $z = L/\xi(T)$ where $L$ is the characteristic finite size of the system and $\xi(T)$ is the correlation length of the bulk system at temperature $T$, completely determines the finite size corrections to bulk behaviour needed to describe the finite system. This assertion can be posed as a statement that the singular part of a thermodynamic property per unit volume of a system close to criticality has the form:

$$P^L(T) \sim L^w Q^T_p(z)$$

(1.66)

where $p$ specifies the thermodynamic function. The distance from pseudo-criticality is given by

$$t' = (T - T_c(L))/T_c$$

(1.67)

and it is expected that the $P^L(T)$ depends on $T$ via $t'$ and $L$ through the amount of rounding as given by equation (1.64). If $\lambda$ and $\theta$ were both $1/\nu$, 

$$\frac{(T_m(L) - T_c)}{T_c} \sim b/L^\lambda$$

(1.63)
then the equation \( \xi(T) \sim |t'|^{-\nu} \) in (1.66) would suggest:

\[
P^T_L(T) = L^w Q^T_p (L^{1/\nu} t')^{\nu},
\]

and hence with a redefinition of \( Q_T \)

\[
P^T_L(T) = L^w Q^T_p (L^\theta t'),
\]

which is a particular example of (1.66). Below a renormalisation group derivation is given for equation (1.69). For the time being it is assumed to hold even if the assumption \( \theta = 1/\nu \) and \( \lambda = 1/\nu \) is relaxed.

The implications of equation (1.69) are now investigated for a system exhibiting pseudo-critical behaviour. The analysis for a finite system with true critical behaviour is given in Barber (1983). In particular the exponent \( w \) in (1.69) can be related to a standard bulk exponent as follows. Suppose that macroscopic thermodynamic functions are observed to exhibit power law like divergences (as in table (1.1)):

\[
P^\infty _T (T) \sim C_\infty t'^{-\rho}.
\]

Equation (1.69) should recover this result as the bulk limit is taken and so

\[
\lim_{L \to \infty} P^T_L(T) = L^w Q^T_p (L^\theta t')
\]

must take some finite value for \( t' \) non-zero. The function \( Q^T_p (z) \) is assumed to have to leading order for large \( z \) a form:

\[
Q^T_p (z) = A z^a (1+B z^{-b}+...); \quad a > 0, b > 0
\]

which when plugged into the limit, (1.71), gives:

\[
\lim_{L \to \infty} P^T_L(T) = A L^w (L^\theta t')^a (1+B (L^\theta t')^{-b}+...).
\]

The powers of \( L \) must cancel to leading order to obtain a finite value.
corresponding to the result (1.69) away from criticality. This implies:

\[ w + a \theta = 0 \quad (1.74) \]

while agreement with (1.70) requires:

\[ a = -\rho \quad (1.75) \]

as \( t' + t \) as a result of \( L \to \infty \) and hence that:

\[ w = \rho \theta \quad (1.76) \]

to give finally,

\[ P^T_L(T) = L^\theta Q^T_{\rho}(L^\theta t') \quad (1.77) \]

as a basis for a finite size scaling analysis of the 3 d Ising model for finite \( L \) and \( t' > 0 \).

Equally, finite size scaling analysis can be applied to quantities measured at pseudo-criticality in equation (1.69) in our finite system. In this case for \( L \) finite and \( t' \to 0 \) the behaviour of \( Q^T_L(z) \), in equation (1.69), is required for \( z \) small. If there is no phase transition but only pseudo-critical behaviour (as in the case of 3 d Ising with periodic boundary conditions), then: \( Q^T_L(z) \to Q^T_0 \) as \( z \to 0 \) and so \( P^T_L \) is a finite number and (1.69) gives:

\[ P^T_L(T \to T_c(L)) \sim Q^T_0 L^{D/V} \quad (1.78) \]

which describes how these pseudo-critical properties scale with system size.

Equations (1.77) and (1.78) imply that for finite systems exhibiting rounded pseudo-critical behaviour the finite thermodynamic quantities vary close to and at \( t' = 0 \) with \( L \) in a way determined by the bulk critical exponents. This is the basis of finite size scaling methods of obtaining bulk critical exponents. The use of periodic boundary conditions removes surface effects from the finite system and hence the possibility of cross over from the pseudo-critical behaviour of the \( L^d \) system to that of the \( L^{d-1} \) system embedded in the...
surface.

The above finite size scaling picture follows naturally from Fisher's hypothesis that the finite size correction depend only on the ratio $\xi/L$. This hypothesis can be established using the RSRG formalism. The field theoretic discussion is presented in for example Brezin, Le Guillou and Zinn-Justin (1976) and the real space formalism is reviewed by Barber (1983). We restrict ourselves to a summary of the latter. The starting point is the generalisation of (1.44), recognising that the free energy per spin will depend on the number of degrees of freedom $N'$ but arguing, for a local RSRG transformation, that $g(u_1, \ldots)$ will not depend on $L$, we obtain on iterating $I$ times:

\[
\sum_{j=0}^{I} g(\lambda_1^j u_1, \lambda_2^j u_2, \lambda_3^j u_3, \ldots; b^j L^{-1}) b^{-j I} = f(u_1, u_2, u_3, \ldots; L^{-1}) + b^{-l} f(\lambda_1^j u_1, \lambda_2^j u_2, \lambda_3^j u_3, \ldots; b^j L^{-1})
\]

(1.79)

The first term has no $L$ dependence other than the limit placed on the sum because $I$ must be such that $b^{l} / L$ is less than 1. This of course holds only if the renormalisation transformation is chosen to ensure $g(u \lambda^j)$, the contribution to the free energy from the integration over length scales $b^{j-1}$ to $b^j$ in lattice units, is not extensive. Provided the restriction on $I$ is not too severe then the finite size dependence resides with the residual term $b^{-l} f(\lambda_1^j u_1, \lambda_2^j u_2, \lambda_3^j u_3, \ldots; b^j L^{-1})$ which bears the brunt of the boundary conditions. Clearly, $1/L$ can be thought of as an additional relevant scaling field since its exponent is greater than zero. The analysis of Niemeijer and van Leeuwen (1976) which gave (1.48) now gives with the inclusion of $L^{-1}$ as an extra relevant scaling field the finite size modified homogeneity relation:

\[
f_{\text{sing}}(u_1, \ldots; L^{-1}) = b^{-l} f_{\text{sing}}(\lambda_1^j, \ldots; b^j L^{-1}).
\]

(1.80)

Specifically, iterating $I$ times (as we did to obtain (1.48)) implies a scaling form

\[
f_{\text{sing}}(u_1, \ldots; L^{-1}) = b^{-l I}
\]
Choosing $I$ so that $b^I = L$ we obtain finite size equivalent of (1.48):

$$f_{\text{sing}}(b^I u_1 \ldots b^I L^{-1})$$

Choosing $I$ so that $b^I = L$ we obtain finite size equivalent of (1.48):

$$f_{\text{sing}}(u_1 \ldots : L) = |u_1|^{-d/\gamma_1}$$

$$A_1^{\pm}(u_2 / |u_1|^\gamma_2 / \gamma_1, u_3 / |u_1|^\gamma_3 / \gamma_1 \ldots : L^{-1} / |u_1|^{-1/\gamma_1})$$

(1.82)

The identification $\gamma_1 = \gamma$ and $u_1 = t$ confirms the dependence upon $\xi / L$.

1.7. An introduction to computer studies of phase transitions

The idea that a computer can be given the rules which are thought to characterise the behaviour of a system and can then numerically apply these rules to the numerical equivalent of the degrees of freedom of the system in order to emulate its behaviour, is called computer simulation. The beauty of the computer simulation is that the nature of the degrees of freedom where they reside in the system, the spatial and temporal extent of the system, the boundary conditions and the interaction Hamiltonian can all be precisely controlled. A second nice feature is that any measurement of degrees of freedom and various functions of these degrees of freedom can be made. These two features make the computer simulation a perfect numerical laboratory where the implications of theoretical models can be studied and their characteristic features observed.

The sum in equation (1.9) consists of $2^N$ terms for an Ising spin system ($q^N$ for a system with $q$ states per degree of freedom) which represents exponential increase in the number of configurations with the size of the system. In view of this it is not possible to enumerate equation (1.7) by calculating $A(\sigma)$ for each possible configuration and averaging the result for a system of more than $N \sim 30$ degrees of freedom with present computers.

In terms of the $N$ dimensional phase space of a system with $N$ degrees of freedom there are $2^N$ points corresponding to the possible states of the system. In truncating (1.7) which points in phase space can be safely thrown away and what is the error induced by throwing such points away? Such considerations lead to the concept of importance sampling where certain regions of phase space are sampled more than others in evaluating (1.7).
Randomly sampling the totality of configurations is a specific example where the whole of phase space is taken to have the same importance.

The Monte Carlo method [Binder (1979)] provides a means of estimating an ensemble average such as equation (1.7). The sum over all points in phase space weighted by the correct probability is transformed to an arithmetic sum over a sample of points (configurations) in phase space where each point appears in the sample with a frequency \( P(\sigma) \), that is according to its importance to the ensemble average.

In practice, starting with a configuration \( \sigma(0) \) a Monte Carlo algorithm is used to generate a sequence of configurations:

\[
\sigma(1), \sigma(2), \sigma(3), \sigma(4), \sigma(5) \ldots \sigma(n)
\] (1.83)

such that for \( n \) sufficiently large \( \sigma(n) \) appears with a relative probability \( p_{eq}(\sigma(n)) \). The equilibrium statistical properties of Hamiltonian \( H(\sigma) \) follow from equation (1.9). With no constraints on \( H(\sigma) \), \( p_{eq}(H(\sigma)) \) produces the canonical ensemble. Other ensembles arise when conservation laws are fed in e.g. the microcanonical ensemble when energy conservation is imposed. Arguments that the Monte Carlo scheme is possible, that there exists at least one algorithm which can realise the scheme now follow.

How can it be ensured that if \( p_{eq}(\sigma) \) is reached the algorithm designed to produce configurations with this frequency will continue to do so? Consider a Markov chain or sequence of configurations as shown in (1.83). Let \( p(\sigma(n)) \) be the relative probability with which \( \sigma(n) \) is produced and let \( P(\sigma',\sigma) \) be the probability of the next configuration being \( \sigma' \) if the present one is \( \sigma \). The next application of the algorithm must produce some configuration and so it should be insisted that:

\[
\sum_{\{\sigma'\}} P(\sigma',\sigma) = 1
\] (1.84)

Further if \( P(\sigma',\sigma) \) is to be a probability then:

\[
0 \leq P(\sigma',\sigma) < 1
\] (1.85)

The picture is that \( p(\sigma(t)) \) evolves with MC time (successive applications of the
updating algorithm forming these natural units) hopefully approaching an unique equilibrium probability $P_{eq}(\sigma(t))$ for $t > t_{eq}$ where $t_{eq}$ is a measure of the time for the Markov chain to forget its beginning. This expectation is described by a Master equation:

$$\frac{dtp(\sigma')}{dt} = \sum_{\{\sigma\}} \{P(\sigma',\sigma)p(\sigma)-P(\sigma,\sigma')p(\sigma')\}$$

(1.86)

which says that the amount by which the relative probability of obtaining $\sigma'$ i.e. $p(\sigma')$, changes with time, is the total probability of stepping to $\sigma'$ in the next $dt$ minus the total probability of stepping from $\sigma'$. The requirement for equilibrium is:

$$dp(\sigma')/dt = dp_{eq}(\sigma')/dt = 0.$$ 

(1.87)

One way to ensure that the algorithm remains at $p_{eq}(\sigma)$ if it ever gets there is the over strong condition of detailed balance:

$$P(\sigma',\sigma)p(\sigma) = P(\sigma,\sigma')p(\sigma')$$

(1.88)

which ensures (1.87) holds. Equation (1.88) is a statement that the single Markov steps $\sigma' \rightarrow \sigma$ and $\sigma \rightarrow \sigma'$ are equally likely. A weaker condition is to ensure that $\sigma \leftrightarrow \sigma'$ is equally possible though it may take more than one MC time step.

What other conditions need to be imposed, if any, to ensure that a MC algorithm converges to the probability distribution $P_{eq}(\sigma)$ required? Consider the evolution of the probability $p(\sigma(t))$ before equilibrium is reached. A measure for the difference of any two distributions $p_1(\sigma)$ and $p_2(\sigma)$ is:

$$|p_1-p_2| = \sum_{\{\sigma\}} |p_1(\sigma)-p_2(\sigma)|$$

(1.89)

where the sum is over all possible configurations. The “distance” of the distribution after $n+1$ steps $p_{n+1}(\sigma)$ from the desired $p_{eq}(\sigma)$ is:
\[ |p_{n+1} - p_{eq}| = \sum_{\xi} (|p_{n+1}(\sigma') - p_{eq}(\sigma')|) \]  

but

\[ p_{n+1}(\sigma') = \sum_{\xi} P(\sigma',\sigma) p_n(\sigma) \]

and so

\[ |p_{n+1} - p_{eq}| = \sum_{\xi} (|\sum_{\xi} P(\sigma',\sigma) p_n(\sigma) - \sum_{\xi} P(\sigma',\sigma) p_{eq}(\sigma)|) \]

\[ |p_{n+1} - p_{eq}| = \sum_{\xi} (|\sum_{\xi} P(\sigma',\sigma)(p_n(\sigma) - p_{eq}(\sigma))|). \]

\( (p_n(\sigma) - p_{eq}(\sigma)) \) is sometimes >0 and sometimes <0 and \( P(\sigma',\sigma) > 0 \) therefore:

\[ |p_{n+1} - p_{eq}| < \sum_{\xi} (|\sum_{\xi} P(\sigma',\sigma)(p_n(\sigma) - p_{eq}(\sigma))|) \]

which after interchanging the order of the \( \sum \)'s over \( \{\sigma'\} \) and \( \{\sigma\} \) and using (1.84) becomes:

\[ p_{n+1} - p_{eq} < |p_n - p_{eq}| \]

With successive steps then the probability distribution can only get nearer than it presently is to the equilibrium distribution. The equality only occurs if \( p_n \) is already equal to \( p_{eq} \). The \( \sum \)'s over all configurations used assume that (in an infinite number of steps) the MC algorithm has a finite probability of accessing every microstate of the system in principle, that it neither gets trapped in a portion of phase space nor oscillates between portions and never visits others. These issues and that of ergodicity and mixing are discussed further in Bhanot et al. (1984) and Kennedy et al. (1984).

**Implementations of Monte Carlo**

There remains a lot of freedom within the detailed balance condition (1.88) and conditions (1.84) and (1.85) for choosing the rule for obtaining the next
configuration $\sigma'$ from $\sigma$ with transition probability $P(\sigma',\sigma)$. Where possible this freedom is exploited to maximise the, the rate of equilibration, the rate at which spin correlations are diffused.

The Metropolis algorithm (Metropolis et al (1957)) implements a MC update by performing many single spin flips. The advantage of this is that the transition probability depends only on local pattern of spins connected to the spin being updated through the Hamiltonian with the added advantage of being easily adapted for parallel updating. The general updating cycle is choose one spin of the lattice say $\sigma_i$ of configuration $\sigma$. Pick a trial value for this spin. Calculate the energy change $\Delta H = H(\sigma') - H(\sigma)$. If $\Delta H > 0$ accept the trial spin $\sigma'_i$. If $\Delta H < 0$ accept the trial $\sigma'_i$ with the probability $\exp(-\Delta H)$ (that is if $\exp(-\Delta H) >$ a pseudo-random number normalised to the range 0 to 1 accept the trial state) otherwise keep the old spin $\sigma_i$. Repeat the procedure for all spins of the lattice which can be visited randomly or regularly. One update of the whole lattice is called a sweep or MC step. The detailed balance condition is respected by this algorithm as can be verified.

When considering simultaneously updating spins by means of the local energy changes, the detailed balance condition requires that spins connected through the Hamiltonian are not updated at the same time.

1.8. Research Projects

In chapter 2, hyperscaling is reviewed and possible violations of it in the 3d Ising model are considered. The details of such tests performed at Edinburgh involving extensive MC simulations achieving very high statistics made possible using state of the art fast Metropolis code are presented together with particulars of implementing such a computer experiment on the I.C.L. Distributed Array Processor (DAP). A careful analysis of the data to eliminate the dependence on the starting configuration and to faithfully assess the MC statistical errors together with a finite size scaling interpretation of the resulting ensemble estimates for the various quantities measured is presented. The value obtained for the critical exponent $\nu$, Fisher's anomalous dimension, establishes agreement with Fisher and Chen (1985). The large systems and high statistics allow an accurate estimate of $\nu$ not dependent on assumptions about corrections to scaling. Hyperscaling is seen not to be violated. Estimates for $\alpha, \beta, \gamma, \Delta$ and $\nu$ are in accord with the sophisticated analysis of Fisher and Chen of Nickel's (1980) correlation length and susceptibility series.
The RG formalism naturally predicts hyperscaling will hold and as yet has only been extended to furnish a theoretical argument for its violation where the inclusion of dangerous irrelevant scaling fields can be justified. There being no evidence for dangerous irrelevant fields in the three dimensional Ising model the validity of hyperscaling suggests the that the identification (1.52) to (1.55) between $\gamma_r$, $\gamma_h$ and the critical exponents do not require modification.

In chapter 3 the Monte Carlo Renormalisation Group (MCRG) method is reviewed and extensions to the method of analysis due to Wilson and Swendsen are introduced. The MCRG data of Pawley et al (1984) is analysed to study coupling constant flow. The conclusions touch on some of the limitations of MCRG, and on possible improvements.

Chapter 4 is concerned with attempts to improve MCRG and starts by reviewing the most recent suggestions for optimisation. Swendsen's optimised MCRG (OMCRG) is implemented and the results presented. The conclusions raise many questions over the practical progress of this approach to date.

Use of the microcanonical ensemble in the simulation of systems near criticality and a review of recent work on the Demon methods of Creutz are the subject of chapter 5. The main achievements of this work to date are the development of exceptionally fast algorithms, updating roughly $10^9$ spins per second on the DAP. The potential of the demon methods and Metropolis methods of estimating canonical ensemble averages are investigated.

At the end of chapter 5 we spell out the conclusions of the research work presented in chapters 2, 3, 4 and 5 and suggest research which might be of interest.
NUMERICAL TESTS FOR HYPERSCALING VIOLATION

IN THE THREE DIMENSIONAL ISING MODEL

2.1. Introduction

The RG formulation of critical phenomena and the correlation length scaling hypothesis naturally give both the ordinary (1.55) and the hyperscaling (1.56) relations between critical exponents, the latter characterised by the inclusion of at least one thermal and one correlation exponent and the dimensionality d. A violation of hyperscaling would indicate the need for an extension of the RG formulation of critical phenomena and the correlation length scaling hypothesis to incorporate it. The inclusion of "dangerous" irrelevant scaling fields [Fisher (1983)] provides a possible mechanism by which RG can incorporate hyperscaling violation. In the Ising model in three dimensions there is no evidence for such "dangerous" scaling fields to date, consequently a violation here would make further demands on the RG formulation of critical phenomena. Before using the RG formalism on the three dimensional Ising model, as I do in chapters 3 and 4, it is appropriate to test the validity of hyperscaling. And so in this chapter recent numerical tests of hyperscaling are reviewed. A particular test of hyperscaling involving MC simulation of the three dimensional Ising model and the theory of Finite Size Scaling, carried out at Edinburgh, is presented. Some detail is included concerning MC refinements and the implementation of fast algorithms using the Distributed Array Processor (DAP). A careful analysis of the numerical data produced by such a computer experiment is made and the results discussed in comparison with recent work by Freedman and Baker (1982), Barber et al (1983), Binder et al (1984) and Fisher and Chen (1985). The conclusions and implications for the RG formulation of critical phenomena and for the correlation length scaling hypothesis are then discussed.
2.2. What is hyperscaling?

The hyperscaling hypothesis is that the so-called hyperscaling relations (1.56) hold as well as the ordinary relations (1.55). The ordinary scaling relations are found to hold for all soluble models to date, including the spherical model for general d. The hyperscaling relations hold for the two dimensional Ising model but are known to fail for d > 4; for example in the spherical model \( w^\alpha \nu = d \nu - (2-\alpha) = 1/2(d-4) \), or e.g. the d = 5 Ising model [Binder et al. (1984)]. In the three dimensional Ising model work prior to 1980 suggested hyperscaling failed [Domb (1974)]. The MC work of Freedman and Baker (1983) gave a non-perturbative estimate of Fisher’s anomalous dimension, \( w^\alpha = 0.20(8) \), which they interpreted as a violation of hyperscaling. Fisher and Chen (1985) have performed a sophisticated analysis of the susceptibility and correlation length series data of Nickel (1980) for \( \gamma, \nu \) and \( \alpha \) in the double-Gaussian and Klauder models in d = 3. These models interpolate, as a function of \( \gamma \) (a factor in the single spin weight function), between the pure Gaussian model (\( \gamma = 0 \)) and the spin one half Ising model (\( \gamma = 1 \)). Tuning to \( \gamma_c \) where the effects of non-analytic corrections to scaling are minimised they find \( w^\alpha \nu = d \nu - (2-\alpha) = 0.001(10) \), giving positive support for the validity of hyperscaling in three dimensional scalar spin models, independent of assumptions about non-analytic corrections to scaling. They suggest that apparent violations seen in the pure three dimensional Ising model are attributable to small but significant non-analytic corrections to scaling. Here we repeat the MC test performed by Freedman and Baker on the three dimensional Ising model but to higher lattice size and statistics as afforded by state of the art parallel computing. Our results are quantitatively comparable to those of Fisher and Chen, adding MC support for the validity of the hyperscaling hypothesis in the model.

Possible violations of hyperscaling within the RG framework

To illustrate what constitutes a test of hyperscaling I briefly review how the RG formalism accommodate violation [Binder et al. (1985)] where the inclusion of “dangerous” irrelevant scaling fields [Fisher (1983)] is justifiable. As briefly outlined in chapter 1 the RG formulation of finite size scaling gives the finite size scaling relation for the singular part of the free energy as,
\[ f_L(t,h,u) = L^{-d} f(tL^Y_t,hL^Y_h,uL^Y_u), \quad (2.1) \]

and the finite size scaling relation for the singular part of the correlation length as

\[ \xi_L(t,h,u) = L \xi(tL^Y_t,hL^Y_h,uL^Y_u), \quad (2.2) \]

where from now on we shall assume \( t, h \) and \( u \) to be small so that (2.1) and (2.2) are valid. As in chapter 1, \( t \) is the reduced temperature, \( t = (T - T_c)/T_c \), \( T \) the transition temperature of the infinite system, \( h \) is the external magnetic field and \( u \) is an irrelevant scaling field (representing the many possible such scaling fields). Corresponding to \( t \) and \( h \) are the relevant scaling RG exponents \( \gamma_t > 0 \), \( \gamma_h > 0 \) while \( \gamma_u < 0 \) represents the effective irrelevant RG exponent. Following Binder et al's work the possibility that \( u \) is a "dangerous" irrelevant variable is parameterised as a simple power law singularity in either or both the universal functions \( f(x,y,z) \) and \( \xi(x,y,z) \) as \( z \to 0 \):

\[ f(x,y,z) = z^{p_1} f(xz^{p_2},yz^{p_3}) \quad (2.3) \]

\[ \xi(x,y,z) = z^{q_1} \xi(xz^{q_2},yz^{q_3}). \quad (2.4) \]

The "dangerousness" of either or both (2.3) and (2.4) can be switched off by setting either or both \( p_1 = 0 \), \( p_2 = 0 \), \( p_3 = 0 \) or/and \( q_1 = 0 \), \( q_2 = 0 \), \( q_3 = 0 \). Taking the limit \( uL^Y_u \to 0 \) and using equations (2.3) and (2.4) implies:

\[ f_L(t,h,u) = L^{-d^*} f(tL^Y_t,hL^Y_h) \quad (2.5) \]

where

\[ d^* = d - p_1 \gamma_u \]

\[ \gamma^*_t = \gamma_t + p_2 \gamma_u \]

\[ \gamma^*_h = \gamma_h + p_3 \gamma_u \]

and
\[ \xi_L(t,h,u) = L^{1+q_1y_u} \xi(tL^{y_u}, hL^{y_h}) \]  \hspace{1cm} (2.6)

where

\[
\begin{align*}
V_t^+ &= V_t + q_2V_u \\
V_h^+ &= V_h + q_3V_u
\end{align*}
\]

and \( y_t^* = y_t^+ \), \( y_h^* = y_h^+ \) in general. The scaling combination \( uL^{y_u} \) is henceforth assumed to be sufficiently small to make \((2.3)\) and \((2.4)\) valid. [Other forms of “dangerous” singularities could be considered .]

Setting \( t \) and \( h \) to be small using the fact that in the bulk limit, \( L \to \infty \), the singular part of the free energy per degree of freedom exists and takes some finite value, then \( f(x,y,0) \) for \( x, y \) large must be such that the powers of \( L \) in \((2.5)\) can disappear to yield

\[
f_{\infty}(t,h,0) = |t|^{d/\gamma_t} A_1^{-1/\gamma_t} (h/|t|)^{-\gamma_h/\gamma_t} \hspace{1cm} (2.7)
\]

which is just the scaling form obtained in chapter 1 equation \((1.48)\) but with “dangerous” modifications to the exponents. Though the dangerous correction to scaling has been absorbed other corrections to scaling not parameterised here may of course be important.

Similarly the correlation length, for \( t, h \) and \( u \) small but non-zero \( \xi_L \), equation \((2.6)\), should tend to a finite number as \( L \to \infty \), which requires that the powers of \( L \) disappear in equation \((2.6)\) in this limit and hence the general form:

\[
\xi_{\infty}(t,h,0) = |t|^{(1+q_1y_u)/\gamma_u} B_1^{-1/\gamma_t} (h/|t|)^{-\gamma_h/\gamma_t} \hspace{1cm} (2.8)
\]

The various finite size thermodynamic quantities of interest can be obtained for \( uL^{y_u} \to 0 \), by taking suitable derivatives of the free energy, equation \((2.5)\), and taking the limits \( h \) and \( t \) going to zero, exactly as was done in chapter 1 for the non-“dangerous” case. Similarly the correlation length exponent \( \nu \) and the correlation function decay exponent, \( \eta \), can be related to the RG exponents. Taking the bulk limit of the resulting quantities or using \((2.7)\) and \((2.8)\) as a starting point and taking suitable derivatives, the critical exponents can be related to: the renormalisation group exponents \( y_t, y_h, y_u \); the
"dangerous" corrections $p_1$, $p_2$, $p_3$, $q_1$, $q_2$, $q_3$, and the dimensionality $d$ and $d^*$. The relationships resulting from the above are:

\[ \beta = \frac{(d^*-v_+^*)}{v_t^*} \]
\[ \gamma \pm = \frac{(d^*-2v_+^*)}{v_h^*} \]
\[ \delta = \frac{v_h^*}{(d^*-v_+^*)} \]
\[ \Delta_n = \frac{v_t^*}{v_h^*} \]
\[ \alpha^\pm = 2-d^*/v_t^* \]
\[ \nu^\pm = \frac{(1+q_1v_u)}{v_t^*} \]

where the $\pm$ corresponds to $t \to 0\pm$. At this point we note that the order of taking the limits $t$ and $h$ to zero and the $L$ going to infinite makes no difference to quantities dependent solely on the free energy or solely dependent on the correlation length. Where hyperscaling is violated this is not true for quantities depending on both the free energy and the correlation length.

Eliminating $V_t$, $V_h$ and $V_u$ from the above equations yields relationships among the critical exponents with "dangerous" corrections included. It is found that regardless of the values of $p_1$, $p_2$, $p_3$ the following, "ordinary", relations exist between thermal and correlation exponents:

\[ \alpha+2\beta+\gamma = 2 \]
\[ \Delta = \beta\delta = \beta+\gamma \]
\[ \gamma = (2-\eta)v \]

all of which are devoid of dimensionality. The first two hold for all $q_1$, $q_2$ and
q_3 while the last one is in general violated if the correlation length and/or function have "dangerous" irrelevant corrections which do not conspire to cancel.

For \( p_1, p_2, p_3, q_1, q_2, q_3 = 0 \) so called hyperscaling relations are guaranteed to hold between thermal exponents, \( \alpha, \beta, \gamma, \delta, \Delta \), correlation exponents, \( \nu \) and \( \eta \), and the dimensionality \( d \):

\[
\begin{align*}
\nu &= 2 - \alpha \\
\frac{d(\delta-1)}{(\delta+1)} &= 2 - \eta \\
\nu &= 2\Delta - \gamma.
\end{align*}
\]

The magnitude of the "dangerous" irrelevant violation to each hyperscaling relation when \( p_1, p_2, p_3 \) and/or \( q_1, q_2, q_3 \) are not all zero, is the same for all three relations (with the proviso for the the relation including \( \eta \) that dangerous corrections enter the correlation function finite size scaling relation via \( \xi_l \)) and is given in curly brackets in the equations below.

\[
\begin{align*}
\nu &= 2 - \alpha + \{ \frac{d(1+q_1\gamma)}{(\gamma+q_2\gamma)} - (d-p_1\gamma)/(\gamma+p_2\gamma) \} \\
\frac{d(\delta-1)}{(\delta+1)} &= 2 - \eta + \{ \} \\
\nu &= 2\Delta - \gamma + \{ \}
\end{align*}
\]

all of which depend on \( d \) the dimensionality. The "guarantee" disappears if any of the "dangerous" exponents are non-zero though it is still possible that the "dangerous" corrections conspire to respect some or all of the hyperscaling relations. When the terms \( \{ \ldots \} \) are set to zero, the relationships between thermal and correlation scaling exponents, (2.12) and the dimensionality go beyond the separate existence of correlation scaling and Widom scaling, uniting them into one rule, that constitutes hyperscaling. The extent to which measured or calculated exponents do not satisfy (2.11) indicates the extent to which hyperscaling is violated.
2.3. Tests of hyperscaling in MC numerical work

One approach to testing hyperscaling is to measure the susceptibility, the specific heat, the correlation length etc., by, say a MC simulation, and use the various finite size scaling forms for these observables to estimate the various thermal and correlation critical exponents. Then, with exponent values and errors, the extent to which the hyperscaling relations hold (or do not hold) can be checked. Numerically this is not the best way to proceed because the errors would have to be combined and the correlation between different quantities measured on the same set of configurations could not easily be exploited. A quantity which depends on both thermal and correlation functions is required which is hence a direct measure of the validity of hyperscaling. The renormalised coupling [Freedman and Baker (1982)],

\[ g_{R,FBL}(t,h,u) = \left( \chi^{(4)}_L(t,h,u) \right)^2 L^d \chi^{(2)}_L(t,h,u) \]  

is such a quantity, it is universal if hyperscaling is satisfied, and, as they illustrate from correlation length scaling, the simplest such quantity which tests hyperscaling.

The MC simulation of Barber et al. (1983) measured

\[ g_{R,BL}(0,0,u) = \chi^{(4)}_L(0,0,u)/[\chi^{(2)}_L(0,0,u)^2 L^d] \]

the renormalised coupling, at criticality for different size systems. Setting \( t = 0, \ h = 0 \), for the finite system, where \( t = (T-T_c(L))/T_c \) is understood to be the finite size shifted reduced temperature, before allowing the system size to grow, \( L \to \infty \), thus pushing \( uL^y \) in to the "dangerous" regime, \( g_{R,BL}(0,0,u) \) is seen to scale as:

\[ g_{R,BL}(0,0,u) = L^{-(d-d^*)} \]

\[ \partial^4 f(tL^y_t, hL^y_h)/\partial(hL^y_h)^4 \]
They found \( d-d^* = 0.00 \pm 0.04 \). This test does not constitute a test of hyperscaling since \( d-d^* \) does not correspond to the "dangerous" violation indicated in the curly brackets of (2.8). Binder \textit{et al.} provided three arguments to support \( d = d^* \) even in instances where hyperscaling is violated (i.e. \( p_1 = 0 \) but \( p_2, p_3 \) non-zero and \( q_1, q_2 \) and \( q_3 \) anything, together with MC data for the five dimensional Ising model.

Freedman and Baker (1983) measured (2.13) for the pure three dimensional Ising model on a simple cubic lattice with periodic boundary conditions. The MC simulation was performed on various size lattices with \( K_{nn} \) tuned to \( K_{nn}^* \) corresponding to a reduced temperature \( t^* > 0 \), such that the correlation length is a fixed fraction of the lattice size i.e. \( \xi(t^*,0,u) = cL \) with \( c \) a constant chosen to be 0.275. With this choice of \( c \) the system is simulated in the regime where on the one hand the rounded finite size curves for divergent quantities such as specific heat and susceptibility agree with the bulk curves i.e. \( t^* \gg (T_m(L)-T_c)/T_c \) (recall (1.64)) and on the other hand as large as possible so that \( L \to \infty \) takes the system to \( t \to 0^+ \) and the scaling region for as small a lattice as possible. Tuning the degree of criticality by monitoring the correlation length also constitutes both a faithful and sensitive measure of the degree of criticality. Simulating in this way so that finite estimates for quantities are rounded and shifted very little with respect to the corresponding bulk quantities (in contrast to a MC simulation performed at \( T_c \)) allows the following finite size scaling analysis to be performed on the interpolated measured quantities. that the \( g_{R,FB,L}(t^*,0,u) \) measured corresponds to taking the bulk limits for each quantity on the r.h.s. of (2.13) before substituting them and then replacing \( t^* \) using:

\[
\xi(t^*,0,u) = cL = |t^*|^{-(1+q_1+y_1)} \xi(t^*L_t^*y_1,0). \tag{2.16}
\]

This gives for the renormalised coupling the scaling form:

\[
g_{R,FB,L}(t^*,0,u) = L^{-w^*}(\delta^2f/\delta(hL_{1n}^*)^2)(aL^{y^*_1-y_1+1+q_1+y_1})\bigg/\]

\[
[\delta^2f(tL_{1n}^*,hL_{1n}^*)/\delta(hL_{1n}^*)^2]\bigg|_{h=0}^0
\tag{2.15}
\]
where

$$w^* = \left[ d - d^*(y'_t/y_t'(1+q_1y_u)) \right]$$  \hspace{1cm} (2.18)

is Fisher's anomalous exponent, \(w^* = (d - (\gamma + 2B))/\nu\), as can be checked by inserting the various relations between critical exponents and "dangerous" modified RG exponents and \(a\) is some constant related to \(c\). The scaling combination \(L_{1-t}^{y_t - y'/y_t'(1+q_1y_u)}\) is assumed to be \(L^0\) i.e. a constant in the Freedman and Baker test which corresponds to insisting that only the free energy has "dangerous" corrections, so that \(q_1, q_2\) and \(q_3\) can be set to zero. This assumption makes the amplitude of \(L^{-w^*}\) in (2.17) a constant. On lattice sizes \(L = 3\) to \(L = 60\) they observed a "systematic downward trend by more than twice the statistical error in a quantity which should be constant if hyperscaling is not violated" and found \(w^* = 0.20(8)\).

Naively one might expect in the limit of \(L\) being sufficiently large that \(K_{nn}^a\) is very close to \(K_{nn,c}\) that Freedman's \(g_{RFB}\) would differ only by a factor \(1/c^d\) with Barber's \(g_{RB}\). This is true in this limit. However the two quantities approach this limit in different ways. In Barber's case the numerical experiment sets \(t(L)L_{1-t}^{y_t^*}\) to zero (by setting \(T = T_c(L)\)) then \(L\) to infinite, so that \(tL_{1-t}^1\) and \(t\) are constant, i.e. zero, throughout the whole experiment for all the lattice sizes used. In Freedman's case the numerical experiment takes \(L\) to infinite whilst keeping \(tL_{1-t}^1\) constant, i.e. the effective distance from criticality and the finite size effects remain constant, but for them \(t\) approaches zero as \(L^{-y_t^*}\). This is the crucial difference between the two methods which accounts for the different exponents measured.

At Edinburgh we have repeated the test used by Freedman and Baker but have simulated on \(L = 2, 4, 8, 16, 32, 64\) and 128 obtaining very high statistics. The hope has been that the larger lattices will, in reducing the scaling combination \(uL_{1-u}^{y_u}\), reduce the amplitude of the corrections to scaling, allowing a careful fit to find \(w^*\) rather than some average of correction to scaling exponents.

Summarising we have seen that within the RG formulation of thermodynamic and correlation function finite size scaling the existence of "dangerous" irrelevant scaling fields parameterised as power-law like divergences specified...
by $p_1$, $p_2$, $p_3$, and or $q_1$, $q_2$, $q_3$ might lead to violations of hyperscaling of a kind which can be accommodated within the RG formulation. Within this formalism measurement of $w^* = (d/v - (y+2B))/v$ is seen to be the most direct test of hyperscaling, $w^* = 0$ corresponding to the validity of hyperscaling and $w^* = 0$ quantifying the magnitude of the violation.

2.4. Computational aspects of the MC test on the ICL distributed array processor

The hyperscaling test chosen requires good estimates for the canonical averages on systems of linear dimension $L = 2$ to $L = 128$ each at several temperatures in order to interpolate to $K_n^*$ corresponding to $t^*$ for which $\xi_L(t^*, 0, u)/L = 0.275$. The large systems and high statistics required make heavy demands on both the configuration generation algorithm and the measurement algorithm. These demands are met by exploiting hardware features of the DAP which is described briefly below. More comprehensive descriptions are to be found in Reddaway et al (1985) and references therein.

**The DAP**

The International Computers Limited (ICL) Distributed Array Processor (DAP) is an example of a Single Instruction Multiple Data (SIMD) parallel processing computer. This means that the machine can simultaneously (synchronously) perform the same operation on many different numbers.

The DAP hardware consists of what can be thought of as a square array of 64 by 64 bit-serial processors each connected to its 4 nearest neighbours in hardware. Data can be passed between processors via these nearest neighbour connections which is very important for shift operations. The 4096 processors can be thought to constitute a plane. Each processor has "above" it 4096 logical bits of memory (so the DAP plane has 4096 store planes of memory "above" it) in which the instructions controlling the processors and the data on which they are to act, are stored. The machine therefore has a total of 2 Megabytes of memory.

Three planes are reserved for processing: the Q (sum), C (carry) and A (activity). The activity plane is used to prevent results being written to the indicated sites in a plane (Q, C or addressed), thereby preserving this site's
contents where the A-plane has a .FALSE. or zero bit. In this way logical masks can be created as source code (DAPFORTRAN or APAL) and used to indicate elements of a 64 by 64 array of data which are not to be written to with the result of the present instruction. This masking out of unwanted results together with the nearest neighbour connections are the key features that allow the DAP to do more interesting computing than simply 4096 serial processors working in the same way on different data.

There are two ways at present to program the DAP corresponding to the languages DAPFORTRAN and APAL. DAPFORTRAN, as the name suggests, is a "parallel" extended version of FORTRAN. APAL consists of assembly code instructions and allows more direct programming of the DAP and hence greater exploitation of particular DAP features. As a general rule DAPFORTRAN and existing algorithms are sufficient for most problems with REAL and/or INTEGER*1,2,3,4,5,6,7 and 8 variables together with logical matrices. For logical operations and numbers smaller than $2^7$ i.e. in the region $-2^7...2^7-1$ it can be worthwhile using an optimised program written in APAL, especially if a particular operation is performed many times. Such a situation arises in Ising spin problems particularly where the logical nature of the Ising spin lends itself readily to the DAP's structure and it is well worth while writing fast code in APAL. Such programs for generating Ising configurations for three dimensional simple cubic lattices of $L = 64$ and 128 [Reddaway et al (1985)] together with fast random number generators have been written [Smith et al (1985)] the 128 routine updating spins at 219 million spin update attempts per second. We believe this to be faster than any equivalent program on a vector processor to date. Further features of the DAP will be exposed by describing the DAPFORTRAN version of the hyperscaling program first used. Comments on APAL are postponed until chapter 5.

**Mapping various sizes of Ising model onto the DAP**

Consider for simplicity $64^3$ Ising spins on a simple cubic three dimensional lattice with periodic boundary conditions. The spins, ±1, are represented in the DAP as .TRUE. for +1 or "up" and .FALSE. for -1 or "down". Hence 64 logical planes can be taken to represent 64 planes of Ising spins. The periodic boundary conditions are provided free by the hardware connecting processors at one edge to that at the other as requested. For example, the DAPFORTRAN
instruction SHNC(A(,),2) which shifts the 64 by 64 array A(,) globally two steps to the "North" on the PE. matrix the north most two rows being shifted into the south most two rows. In the 3rd direction the program must look after the periodic boundary conditions.

For systems smaller than $L = 64$ by factors of 2, configurations are interleaved and several simulations are conducted in one run. This makes for ease of programming, avoids having eager processors standing idle and increases statistics. For $32^3$, 4 configurations are updated in parallel and are stored as shown in figure (2.2).

For systems smaller than $L = 64$ by factors of 2, configurations are interleaved and several simulations are conducted in one run. This makes for ease of programming, avoids having eager processors standing idle and increases statistics. For $32^3$, 4 configurations are updated in parallel and are stored as shown in figure (2.2).

The beauty of interleaving configurations is that it allows the same code to be used with minor alterations such as shifting by multiples of 2 for $L = 32$ and multiples of 4 for $L = 16$ etc. The table below shows the shifts required for different system sizes.

<table>
<thead>
<tr>
<th>System Size</th>
<th>Shift Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$32^3$</td>
<td>2</td>
</tr>
<tr>
<td>$16^3$</td>
<td>4</td>
</tr>
<tr>
<td>$8^3$</td>
<td>8</td>
</tr>
<tr>
<td>$4^3$</td>
<td>16</td>
</tr>
<tr>
<td>$2^3$</td>
<td>32</td>
</tr>
</tbody>
</table>

It is of course crucial to keep these interleaved configurations separate and not to mix during updating. Measurements must also take account of the interleaving.

The mapping used for $L = 128$ is rather different. The $128^3$ spin configuration can be divided into $2^3$ cells each of which has 8 spins in it. All the points corresponding to a given position in the cell are stored in 64 bit planes, similarly the other 7 types of point in the cell. In this way $128^3$ is
divided into 8 sets of $64^3$ storage areas 1 for each corner of the $2^3$ nearest neighbour cube. This mapping is generalisable to all lattice sizes $L = 64^n$ where $n$ is an integer greater than 1, simply by increasing the unit cell to be $n^3$ but similarly numbering the points inside.

**Configuration generation**

For the Ising model, nearest neighbour spins are connected through the Hamiltonian and so a logical mask similar to a checkerboard must be used to ensure only non-interacting spins are simultaneously updated and the detailed balance condition satisfied. Such a logical mask where .TRUE. defines the spins subject to updating in this plane.

A further refinement is to note that the plane below has a "negative" checkerboard of spins which do not interact with the chosen subject spins of the present layer. Thus though only half of each plane may be simultaneously updated no DAP processors need be wasted if say, successive planes are correctly merged together to form an updateable plane. After updating or at least before measuring merged planes can be de-merged, the spins going back to their respective planes to recover the physical storage of spins. For more complicated Hamiltonian fewer spins per plane can be simultaneously updated, but with a more complex logical mask a complete updateable plane can be formed by merging a sufficient number of non-interacting spins from different planes. Again once updated the spins can be de-merged to their more physical addresses. In practice, there is in fact no need to demerge the planes during the simulation. The DAP can therefore be run at 100 % efficiency even for more general models.

**The parallel Metropolis algorithm**

The Metropolis algorithm specifies that a trial configuration be accepted with probability 1 if $\Delta H = H(\sigma_{\text{trial}}) - H(\sigma_{\text{present}}) < 0$ (i.e. if the trial state has a lower energy than the present state) and with probability $\exp(-\Delta H)$ if the trial state has a higher energy than the present state. A Metropolis update of an updateable plane can be realised in DAPFORTRAN, the basic code is:
c declare logical matrices
LOGICAL LSPIN(,,64),LMASK(,,),LUPDATE(,,)
LOGICAL L1(,,),L2(,,),L3(,,),L4(,,),L5(,,),L6(,,)
LOGICAL LNNPLANE(,,),LNNUP(,,),LNNDOWN(,,)
INTEGER*1 NN(,,)
REAL*4 DELTAH(,,)
c merge two planes to make a completely updateable plane
c first create a checkerboard mask using:
c alt(1) = odd rows true even rows false
cc altc(1) = odd columns true even columns false
LMASK(,,) = ALTR(1).LEQ.ALTC(1)
c merge the two sublattices using lmask into lupdate
LUPDATE(,,) = MERGE(LSPIN(,,LAYER),LSPIN(,,LAYER+1),LMASK)
c by now lupdate = lspin(,,layer+1) for lmask false
c and lupdate = lpsin(,,layer) for lmask true
c correctly load lnnplane so nearest east west nn needed
to update lupdate are there.
LNNPLANE = MERGE(LSPIN(,,LAYER+1),LSPIN(,,LAYER),LMASK)
c similarly for the nn above
LUPNN = MERGE(LSPIN(,,LAYER+1),LSPIN(,,LAYER+2),LMASK)
c and the nn below
LNNDOWN = MERGE(LSPIN(,,LAYER-1),LSPIN(,,LAYER),LMASK)
L1 = LUPDATE.LEQ.SHEC(LNNPLANE,1)
L2 = LUPDATE.LEQ.SHWC(LNNPLANE,1)
L3 = LUPDATE.LEQ.SHNC(LNNPLANE,1)
L4 = LUPDATE.LEQ.SHSC(LNNPLANE,1)
L5 = LUPDATE.LEQ.LNNUP
L6 = LUPDATE.LEQ.LNNDOWN
NN = A03ADDPANELES1(L1,6)
c nn now contains the number of nearest neighbours
c for each of the spins in lupdate(,) in such
c a way that nn(i,j) corresponds to spin lupdate(i,j).
NN = 2*NN-6
c nn(i,j) = \sum \sigma_{\text{present}} \sigma_{\text{nn}}
DELTAH = -2K*NN
c compare transition probability with real*4
c random number generator random normalised to lie
c the range 0 to 1.
LUPDATE = LUPDATE.LNEQ.(EXP(DELTAH).GT.RANDOM(0))
LUPDATE now updated
c the updated plane should now be demerged back into
c lspin(,,layer) and lspin(,,layer+1)
c ready for when these planes are updated again.
LSPIN(LMASK,LAYER) = LUPDATE
LSPIN(.NOT.LMASK,LAYER+1) = LUPDATE
c over write lspin(,,layer) with
lupdate wherever lmask is true
c over write lspin(,,layer+1) with
lupdate wherever lmask is false

One complete MC step of a configuration is obtained by updating half of
each plane on the first sweep through the L layers and then updating the
remaining half of the configuration on a second sweep through the L layers. As discussed above updating is actually performed in each sweep on merged planes to ensure each processor is active when performing expensive nn sums, assigning probabilities for the transition to the trial state and for realising these by comparison with a real*4 random number.

This code can easily be improved upon for the Ising Model because there are only a finite number of possible values which ΔH can take and a look-up table can therefore be constructed. Also, rather than calling the transition probabilities conditionally by comparing the integer*1 NN(,) (a matrix of 64 by 64 elements) with the integers 0, 1, 2, 3, 4, 5 and 6, a faster method can be constructed by logical operations on the nearest neighbour spins.

To extend the hyperscaling experiment to larger L requires very fast code to offset critical slowing down and the increased spatial correlations. It is these requirements that prompted considerable effort into producing a fast APAL Ising configuration updating routine. The original ideas for the approach which this implementation uses and for the first piece of code are due to Reddaway, Smith and Scott (1985). The successful "debugging" and testing, which has involved some modification of the original code have been my contribution. This code and modifications to it for further speed up are discussed in chapter 5.

Pragmatic test of the random number generator G05FAST

An essential part of the speed up is the implementation of a very fast pseudo-random number generator called G05FAST [Smith et al (1985)]. Modifying the very fast Ising code of Reddaway et al (1985) appropriately for the two dimensional Ising model for various L=2, 4, 8, 16, 32, 64 and 128 allowed a pragmatic test to be made on the quality of G05FAST comparing the MC averages resulting from a long simulation [Toral and Wall (1986)] with the exact results of Ferdinand and Fisher (1969). As indicated in table (2.1) below the agreement is very good for numbers of calls to G05FAST exceeding 300,000,000, each call generating a 24 bit unsigned random integer.
Table (2.1): Exact and MC results for the $d = 2$ Ising model using G05FAST.

The above results are very encouraging for G05FAST and indicate that any imperfections in it are not going to bias MC estimates for 300,000,000 calls to G05FAST and maybe more. In the hyperscalirig experiment we used G05FAST in the same way as in the $2d$ test, i.e. to generate 24 bit unsigned integers for use in the spin update, although an order of magnitude more calls were made.

**Measurements**

The quantities required for the hyperscaling test are: the zero field susceptibility $\chi^{(2)}_L$, the 4th magnetic cumulant $\chi^{(4)}_L$ and the correlation length $\xi_L$. In addition we chose to obtain: the nearest neighbour interaction $S_{nn,L}$, the specific heat $C_L$ and the magnetisation $m_L$. These are the basic set of measurements made. Care must be taken when measuring the correlation length on a finite lattice. We use the estimate of the correlation length used by Freedman and Baker (1983)

$$\xi_{FB,L}(k) = (\langle S(0)^2 \rangle - \langle S(k)^2 \rangle - 1) / |k|^2$$  \hspace{1cm} (2.19)

where

$$S(k) = \sum_\chi \sigma(\chi) \exp(-ik\cdot\chi)$$

and $k$ is chosen to be the smallest wavevector allowed by the lattice i.e. $2\pi/L$ which was first used by Cooper et al (1982). This definition is much cheaper than the rather direct approach which is to calculate
\[
\xi_L = \sum_{i,j}(i-j)^2\langle\xi_i - \langle\xi\rangle\rangle(\xi_j - \langle\xi\rangle) > \]

\[
\sum_{i',j'}\langle\sigma_i - \langle\sigma\rangle\rangle(\sigma_j - \langle\sigma\rangle) >
\]

(2.20)

involving all possible shifts between all planes in order to calculate \(<\sigma_i\sigma_j>\). In the limit \(L \to \infty\) both measures of the correlation length (2.20) and (2.19) become equivalent.

There is a choice, in using the definition of the correlation length (2.19), between measuring for the smallest \(k\) allowed or measuring for a set of \(k=2\pi n/L\) with \(n=1,2,\ldots,10\) say, and plotting \(<S^{-2}(k)>^{-1}\) versus \(k^2\) and extrapolating to \(k=0\). Substituting the extrapolated value reduces the truncation correction implicit in (2.19). We tried this approach for \(L=64\) and found that indeed

\[
<S^{-2}(2\pi n/L)>^{-1} = \chi^{(2)-1} + A.n^2
\]

where \(A\) is the slope of the plot and \(\chi^{(2)-1}\) the intercept. Substituting into (2.19) gives

\[
\xi^2(k) = \chi^{(2)} + O(K^2)
\]

The difference between the estimates for \(K_{nn}=0.2209\) was as follows: \(\xi^2(2\pi/L)=310.2(10)\) and \(\xi^2(0)=302.5(12)\) for 3,360,000 MCS/S. With system size the effect should scale as \(L^{-2}\) and so might be treated as a finite size correction to scaling. This is what we elected to do in order to avoid the substantial cost of measuring 3 or 4 Fourier transforms. We must, of course, bear in mind that the interpolation to \(\xi(2\pi/L,t^*,0,u^*)\) has this added finite size correction.

The raw measurements required to obtain the above quantities are:

\[
<M>, <M^2>, <M^3>, <M^4>,
\]

\[
<S^2(2\pi q/L) > = \langle\sum_{i,j,k} \sigma_{i,j,k} \exp(-i2\pi qk/L) \{...\}^*\rangle
\]

where \(^*\) indicates complex conjugation.
\[ <\text{Re}(S(2\pi q/L))> = <\text{Re}(\sum_{i,j,k} \sigma_{i,j,k} \exp(-i2\pi qk/L))> \]
\[ <\text{Im}(S(2\pi q/L))> = <\text{Im}(\phantom{.})> \]  

(2.21)

With these quantities measured quantities of physical interest can be estimated such as:

\[ \chi^{(2)}_{L}(t,0,u) = L^{-d}(\langle M^2 \rangle - \langle M \rangle^2) \]

\[ \chi^{(4)}_{L}(t,0,u) = L^{-d}(\langle M^4 \rangle - 4\langle M^2 \rangle \langle M \rangle + 12\langle M^2 \rangle \langle M \rangle^2 - 6\langle M \rangle^4) \]

\[ \xi_{F,B,L}^{2}(2\pi q/L,t,0,u) = \]

\[ \langle S(0)^2 \rangle / \langle S(2\pi q/L)^2 \rangle - 1 \rangle / (2\pi q/L)^2 \]

\[ g_{R,F,B,L}(2\pi q/L,t,0,u) = (\chi^{(4)}_{L}(t,0,u) / (\chi^{(2)}_{L}(t,0,u))^2)^d \]

\[ (L/\xi(2\pi q/L,t,0,u))^d \]  

(2.22)

For \( t > 0 \) all odd powers of the magnetisation, \( \langle M^m \rangle m \text{ odd} \), become zero statistically and so can be set to zero in connected cumulants. If included these non-zero odd powers reduce the measured variance because of their correlation with the even powers measured on the same ensemble of configurations. Such an inclusion could be justified as a finite size effect and should not alter the ensemble averages but only reduce the noise. The form of \( \xi^2 \) and \( g_R \) mean also that there is statistical cancellation between numerator and denominator which further reduces the noise and makes the \( g_R \) test of hyperscaling particularly effective numerically. Note also that it is the fluctuations in \( g_{R,F,B,L} \) not \( \chi^{(4)}/(\chi^{(2)}L^d)^d \), which are the measure of the error.
since they correctly include the fluctuations in the correlation length and the ratio of the cumulants.

At a minimal extra cost we also measure $<Q S_{nn}>$ for all the above raw quantities here denoted by $Q$. This allows $\partial / \partial K_{nn}$ for each physical quantity to be calculated for use in interpolation analysis later. The time dependent correlation functions $<Q(t+\tau)Q(t)>$ were measured and averaged for all $t$, for $\tau=1, 2, 3$, as a check of time correlations. The quantity

$$\phi_Q(\tau) = [<Q(t+\tau)Q(t)> - <Q>^2/(<Q^2>-<Q>^2)],$$

(2.23)

where $[ ]$ denotes averaging over MC time $t$, starting at 1 and falling to zero as $\tau$ becomes larger than the characteristic relaxation time of $<Q>$, gives a measure of the correlations between successive updates. The fluctuations in $<Q>$ and $\partial <Q>/\partial K_{nn}$ were accumulated throughout the whole numerical experiment and provide a method of estimating, by comparison with the correctly estimated standard deviation, the relaxation times of $<Q>$ and $\partial <Q>/\partial K_{nn}$ respectively.

Where ever possible integer variables were used rather than reals and as short an integer as possible without risking overflow. The moments $<M^n>$ and $<M^n S_{nn}>$ and $<S_{nn}^2>$ consequently were stored as integers and loaded into integer*8 variables when written out for analysis later. The Fourier transform necessitates the use of reals and for safety real*8 was used.

**Efficient measurement of the correlation length**

In order to measure the correlation length, $\xi_{FB,L}(2\pi/L)$, the discrete Fourier transform of the magnetisation per site $<\sigma(x,y,z)>$ (the order parameter for the Ising model):

$$<S(k)> = \sum_{x,y} \sum_{z} \sigma(x,y,z) \exp(ikz)$$

(2.24)

for $k = 2\pi q/L$ with $q = 1$, the smallest non-zero wavevector allowed by the periodic lattice, must be calculated. For programming convenience $k$ and $z$ are taken to lie perpendicular to the DAP plane labelled by $x$ and $y$. Directly this could be evaluated, for $q=1,10$ say, using the lines:
DO 4 n = 1,10
RESTWID(,) = 0.0
IMSTWID(,) = 0.0
STWID(,) = 0.0
4 CONTINUE
DO 5 LAYER = 1,L
M1(,) = MERGE(1,-1,LSPIN(,,LAYER))
DO 6 n = 1,10
RESTWID(,,n) = RESTWID(,,n)+M1(,)*COS(twopi.n.LAYER)
STWID(,,n) = IMSTWID(,,n)+M1(,)*SIN(twopi.n.LAYER)
5 CONTINUE
DO 7 n = 1,10
AR(n) = SUM(RESTWID(,,n))/L**3
AI(n) = SUM(IMSTWID(,,n))/L**3
STWIDDLE(,,n) = STWIDDLE(,,n)+AR(n)**2+IR(n)**2
RSTWIDDLE(,,n) = RSTWIDDLE(,,n)+AR(n)
ISTWIDDLE(,,n) = ISTWIDDLE(,,n)+IR(n)
7 CONTINUE

all matrices are real*8 except M1(,) which
is integer*1 and LSPIN(,,64) which are the
matrices containing the configuration

The parallel COS and SIN functions are very expensive and can be replaced
by a look up table say COSINE(LAYER,n), SINE(LAYER,n). The multiplication by
M1(,) can be replaced for Ising spins by an addition or subtraction to give

RESTWID(,,N)=RESTWID(,,N)+
1 MERGE(+COSINE(LAYER,N),-COSINE(LAYER,N),LSPIN(,,LAYER))

A further saving is made if one uses LSPIN(,,LAYER) to flip the sign bit of a
dummy matrix after it has been loaded with COSINE(LAYER,N). This requires
the use of a DAPFORTRAN EQUIVALENCE statement to ensure that the logical
matrix .LSIGNBIT(,) is the sign bit of COSDUMMY(,) in the following lines of
code:

COSDUMMY(,)=COSINE(LAYER,N)
LSIGNBIT(,)=LSIGNBIT(,).LEQ.LSPIN(,,LAYER)
RESTWID(,)=RESTWID(,)+COSDUMMY,

In this way we replace three real*8 assignments (two are implicit in the
merge) and an addition with two real assignments one addition and one
logical operation. This trick is not possible for integers because they are
stored in two’s complement in the DAP.
The various moments of the magnetisation are obtained simply by storing successive measurements of $M$ and $S_{nn}$ in successive elements of a DAP plane treated as a long vector whose 4096 elements label MC measurement times. When a whole plane has been filled the program calculates the desired moments completely in parallel e.g.

\[
\begin{align*}
M(,,n) &= M(,,1)^n \\
MSNN(,,n) &= M(,,n)SNN(,) \\
VM(,,n) &= M(,,n)^2 \\
\text{VARIANCE}(n) &= \text{SUM}(VM(,,n)).
\end{align*}
\]

**Run parameters**

The number of Monte Carlo steps per site (MCS/s) discarded to ensure equilibration, the the number of sweeps between successive measurements and the total number of sweeps for the whole simulation for a particular lattice size and temperature are indicated below.
A priori the optimal values for these parameters are chosen in principle with the criterion of minimising the run time to obtain $g_{RFB,L}$, the quantity we are most interested in, to an accuracy of 5%. To do this a knowledge of the update time per spin, $t_{up}$, the measurement time per spin, $t_{mes}$, and the standing charges of the optimised code must be combined with known dynamic (for equilibration) and equilibrium (for relaxation) critical behaviour of the Metropolis algorithm and the quantity $g_{RFB,L}$ [see for example Binder (1976)]. The a posteriori estimates for the relaxation time for the magnetisation and the nearest neighbour energy are given in columns 7 and 8 of the above table. These estimates are very crudely made by inverting the relationship [Binder (1976)]:

$$\delta A^2 = \frac{\langle A^2 \rangle - \langle A \rangle^2}{N(1 + 2t_A)}$$  \hspace{1cm} (2.25)

where $\delta A^2$ is the correctly assessed standard deviation in the MC estimate for...
\( \langle A \rangle, \langle A^2 \rangle - \langle A \rangle^2 \) is the MC estimate for the fluctuation in \( \langle A \rangle \), and \( \{1+2\tau_A\} \) is the "inefficiency" factor which would be one if each of the \( N \) updates of the lattice produced a configuration totally uncorrelated from all the others. These numbers indicate that we were sampling too often for \( \langle M \rangle \) and too seldom for \( S_{nn} \). The measurements of auto-correlation functions gave the following estimates for relaxation times for the magnetisation as:

\[
\begin{align*}
L=16; & \quad K_{nn}=0.2152; \quad \tau_{relax}=19.2 \text{ MCS/S}. \\
L=32; & \quad K_{nn}=0.21940; \quad \tau_{relax}=76.1 \text{ MCS/S}. \\
L=64; & \quad K_{nn}=0.220899; \quad \tau_{relax}=218.5 \text{ MCS/S}. \\
L=128; & \quad K_{nn}=0.21400; \quad \tau_{relax}=1260.0 \text{ MCS/S}.
\end{align*}
\]

These numbers confirm qualitatively the expected increase in relaxation times. Interpolation of these numbers to \( t^* \) should allow estimates for the relaxation exponents for each quantity to be measured. We intend to do this in the near future.

**Extraction of canonical averages from MC data**

Firstly the equilibration of the system should be checked and raw data excluded from equilibrium averages for measurements corresponding to \( t< \tau_{eq} \) where \( \tau_{eq} \) is the equilibration time. A plot of raw data versus MC time successively coarse grained was used to check the trends of the data for equilibration effects. "Eyeballing" the data together with a priori estimates gives a rough estimate of \( \tau_{eq} \). Next the totality of data is successively coarse grained in to fewer and fewer larger and larger bins. The analysis of variance on these bins in the regime where the number of bins is large and the number of data points in the bin is large, should give the same variance and hence standard deviation in the sample mean. Plotting the variance of the measurements within a bin (and perhaps averaging the result over all the bins) gives an estimate of the population variance, where each member of the population is the basic unit of raw data (in our case a run average of 4096 configuration measurements separated by 100 sweeps). This population variance should be a constant. For small bins the true population variance will
be under estimated because the population within the bin is correlated and any one bin does not contain a representative sample of the variety of the true population (of all configurations). The relaxation time of the most correlated fluctuation is obtained where the plot becomes flat. This indicates the minimum size for a coarse grained bin to be statistically uncorrelated from other such coarse grained bins.

With the population variance and standard deviation known then a consistency check on $t_{eq}$ is that data should be discarded at the beginning of the run where it differs by more than two standard population deviations from the ensemble average. For large numbers of statistically independent bins the central limit theorem applies and the MC estimate for the true mean is normally distributed.

**Interpolation of averaged data**

The various averages $<A>$ are interpolated to $K_{nn}$ where $<\xi_{L}(K_{nn},0,u)> = cL$ using the quadratic form:

$$y = A + B(\xi-cL) + C(\xi-cL)^2$$

(2.26)

in the chi-squared function

$$\chi^2 = \sum (y - <A>)^2/\text{errorsq}$$

(2.27)

where the sum is over all the temperature values simulated for a particular system size. In fact we have chosen to split the totality of data for each lattice size and temperature into several blocks for which we ascertain the sample mean and standard deviation in that mean (using the t distribution where the number of independent bins in a block is smaller than 10). The block means and standard deviations are then used in the interpolation. Thus we have arranged for the number of degrees of freedom in the $\chi^2$ test to be $-15$ so that $\chi^2$ can be taken to be normally distributed while also feeding in some of the fluctuation in $\xi$. The errorsq term in the denominator was chosen to be
\[
\text{errorsq} = \text{std}(\langle A \rangle)^2 + B^2 \text{std}(\langle \xi \rangle)^2 - 2B \text{cov}(\xi, A)/(\text{nbins})
\]  
(2.28)

which accounts for the error in \( \xi \) and in \( \langle A \rangle \) and the correlation between these two quantities (assuming \( C \) to be negligible). All the interpolations gave \( \chi^2 \) of the order of 1 per degree of freedom. Small scaling of the errors has been performed to ensure the interpolated data all corresponds to the same, 67\%, confidence level and thus will appear with the correct weighting in the \( L \) fits. In the scaling we used

\[
\delta A' \delta A' = \delta A \delta A \text{a}^2 \text{ where } a^2 = \chi^2/f \text{ with } f \text{ the number of degrees of freedom.}
\]

For all the interpolations the chi-squared values indicated the error in the interpolated quantity \( A = \langle A(\mathcal{K}^n) \rangle \), corresponding to a confidence level of \( \sim 67\% \). The interpolation was performed with and without the covariance term which typically when included gave a marginally smaller error in the interpolated quantity. A further consistency check was afforded by fitting simultaneously \( \langle A \rangle \) and \( \partial \langle A \rangle / \partial \mathcal{E}_L \) to the chi-squared function:

\[
\chi^2 = \sum (y - \langle A \rangle)^2 / \text{errorsq} + \\
\sum (y' - \partial \langle A \rangle / \partial \mathcal{E})^2 / \text{derrorsq}
\]  
(2.29)

with \( \text{derror} = \text{std}(\partial \langle A \rangle / \partial \mathcal{E})^2 + C^2 \text{std}(\mathcal{E})^2 \) where we have assumed the covariance term to be negligible. In all cases the interpolated quantities \( \langle A(\mathcal{K}^n) \rangle = A \), obtained via (2.29) and (2.27), agreed within errors. Finally the quantities \( \partial \langle A \rangle / \partial \mathcal{K}_n \) were interpolated in a similar way but not including a covariance term.

2.5. Results

Following the above discussion of the methodology of the simulation, we now turn to a discussion of the results. The following tables give the raw data for each temperature and the interpolated results for \( \xi/L = 0.275 \), for lattice
sizes $2^3$, $4^3$, $8^3$, $16^3$, $32^3$, $64^3$ and $128^3$ for each of the physical quantities for a range of $K_{nn}$ values spanning $\xi/L = 0.275$. The derivatives with respect to $K_{nn}$ and $\xi$ of each physical quantity are also included. Preliminary comments on the raw data are made in the table captions. At the bottom of each table we list also the results for the interpolation to the value $K_{nn}$ corresponding to $\xi/L = 0.275$, which are the input for the hyperscaling and finite size scaling fits. We have checked that the derivatives (with respect to $\xi$) of interpolations agree within errors with the interpolations of the tabulated derivatives. Each data table is followed by a graph of the interpolated data which best exposes the trends.
Caption for table (2.3): The magnetisation. Raw and interpolated data. The magnetisation is seen to be zero to within 2 standard deviations for raw and interpolated quantities. A check of the error analysis is that 67% of the measurements have a magnetisation which is zero within the standard deviation and 33% of the measurements are outwith this. We have checked that the coarse-grained bins are normally distributed as expected for MC data (Doob (1953)).

Caption for table (2.4): The raw and interpolated nearest neighbour interaction per spin. The nearest neighbour interaction is seen to tend asymptotically to $s_{nn,r,\infty}$ which we take to be 0.993728(8) from the data of Pawley et al (1984). To date we have not obtained a reliable estimate for $\alpha$. The specific heat shown has the expected scaling behaviour with $t$ for the large lattices but an error in the normalisation of the specific heat has led to scaling with system size an order of magnitude different from that expected. We are currently taking steps to correct this since an accurate measurement of $\alpha$ would provide an invaluable consistency check on the estimate for $w^*$. 

Caption for figure (2.4) The nearest neighbour interaction per spin. In this plot we have used data of Pawley et al for $s_{nn,L}(t=0,0,u)$ in order to plot $s_{nn,L}(t=0,0,u)-s_{nn,L}(t=0,0,u)$ versus $L$. Plotting $\log s_{nn,L}(t=0,u)-s_{nn,L}(0,0)$ gives a slope $(\alpha-1)/\nu \sim 1.3$ for a quantity whose best estimates indicate it should be 1.414.

Caption for table (2.5): Raw and interpolated estimates for $<S^2>$ The interpolation of $<S^2(2\pi/L)>$ gives a check on the estimate of $\gamma/\nu$ since it scales for a fixed wavevector in the same way as $\chi^{(2)}_L(t^*,0,u^*)=<S^2(t_0)>$.

Caption for figure (2.5): The modulus squared Fourier transform of the magnetisation per spin interpolated to $t^*$ versus $L$. The slope of $\log <S^2>_L$ versus $L$ gives $\gamma/\nu = 1.95$.

Caption for table (2.6): The raw and interpolated susceptibility per spin. 

Caption for figure (2.6): The susceptibility per spin. The slope of the $\log \chi^{(2)}_L$ versus $L$ plot gives $\gamma/\nu = 1.96$. Note the consistency of the scaling with $L$ of $\chi^{(2)}$ and $<S^2>$.

Caption for table (2.7): The raw and interpolated 4th magnetic cumulant per spin.
Caption for figure (2.7): The fourth magnetic cumulant per spin. The slope of the \( \log(\chi^{(4)}_L) \) versus \( \log L \) plot gives \( (\gamma + 2\Delta)/\nu = 6.92 \).

Caption for table (2.8): The correlation length and the temperature, raw and interpolated. The temperature corresponding to \( \xi/L = 0.275 \), given in table (2.8), was obtained using the same interpolation procedure with \( Q = B \). The error in the correlation length dominates in the fit since the error \( \delta B = 0.0000001 \). The second parameter in the \( B \) interpolation gives \( \partial \xi/\partial K \) which we found to be in agreement with the \( \partial \xi/\partial K \) estimate obtained by direct interpolation of \( \partial \xi/\partial K \). The latter is taken to be the better estimate of this derivative and is the value shown in the table.

Caption for table (2.9): The raw and interpolated renormalised coupling per spin. The direct interpolation of \( g_{R,FB,L} \) in the second table gives the best estimate for the standard deviation in the interpolated quantity. The third table gives the best estimate for \( g_{R,FB,L}(t^*,0,u^*) \) obtained using the interpolations of \( \chi^{(4)}_L(t^*,0,u^*) \) and \( \chi^{(2)}_L(t^*,0,u^*) \). These two estimates agree to within one standard deviation.

Both our results and those of Freedman and Baker (1983) are presented. The indication is that apparent violations of hyperscaling seen in MC work are due to the effect of small but significant corrections to scaling. The \( L = 128 \) simulation reduces these effects further and is in accord with the work of Fisher and Chen (1985): the slope of \( \log(g_{R,FB,L}(t^*,0,u^*)) \) versus \( \log L \) giving \( w = \).
0.008(20) where \( w^* \) is Fisher's anomalous exponent.
<table>
<thead>
<tr>
<th>L</th>
<th>m_L</th>
<th>( \partial m_L / \partial K_{nn} )</th>
<th>( \partial m_L / \partial \xi(t.o.u..) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.089391</td>
<td>0.000000</td>
<td>( (97) ) 0.005 (33) 0.081216 (501297)</td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>-0.000019</td>
<td>( (64) ) -0.003 (9) -0.048646 (148759)</td>
</tr>
<tr>
<td>8</td>
<td>0.190000</td>
<td>-0.000036</td>
<td>( (471) ) -0.001 (3) -0.001464 (5398)</td>
</tr>
<tr>
<td>16</td>
<td>0.200000</td>
<td>0.000038</td>
<td>( (257) ) 0.000 (6) 0.000481 (6307)</td>
</tr>
<tr>
<td>32</td>
<td>0.205000</td>
<td>-0.000019</td>
<td>( (845) ) -0.001 (6) -0.000523 (5205)</td>
</tr>
<tr>
<td>64</td>
<td>0.210000</td>
<td>-0.000036</td>
<td>( (1042) ) -0.004 (5) -0.002050 (2864)</td>
</tr>
<tr>
<td>128</td>
<td>0.211000</td>
<td>0.0000372</td>
<td>( (1321) ) -0.009 (6) -0.004496 (1987)</td>
</tr>
<tr>
<td>16</td>
<td>0.215000</td>
<td>0.000103</td>
<td>( (682) ) 0.014 (17) 0.000587 (717)</td>
</tr>
<tr>
<td>32</td>
<td>0.215200</td>
<td>-0.000036</td>
<td>( (585) ) 0.019 (16) 0.000795 (644)</td>
</tr>
<tr>
<td>64</td>
<td>0.215500</td>
<td>0.000093</td>
<td>( (359) ) 0.013 (25) 0.000515 (960)</td>
</tr>
<tr>
<td>128</td>
<td>0.219400</td>
<td>0.0000386</td>
<td>( (1339) ) -0.040 (249) -0.000070 (428)</td>
</tr>
<tr>
<td>256</td>
<td>0.219420</td>
<td>0.0000318</td>
<td>( (705) ) 0.002 (179) 0.000003 (324)</td>
</tr>
<tr>
<td>512</td>
<td>0.219450</td>
<td>0.000083</td>
<td>( (578) ) 0.003 (87) 0.000005 (154)</td>
</tr>
<tr>
<td>1024</td>
<td>0.220880</td>
<td>-0.002585</td>
<td>( (1700) ) -1.491 (2335) -0.000120 (204)</td>
</tr>
<tr>
<td>2048</td>
<td>0.220890</td>
<td>-0.00194</td>
<td>( (836) ) -0.019 (1441) -0.000001 (109)</td>
</tr>
<tr>
<td>4096</td>
<td>0.220896</td>
<td>-0.000292</td>
<td>( (291) ) -0.078 (490) -0.000006 (37)</td>
</tr>
<tr>
<td>8192</td>
<td>0.220899</td>
<td>-0.000553</td>
<td>( (513) ) -0.832 (675) -0.000064 (54)</td>
</tr>
<tr>
<td>16384</td>
<td>0.220902</td>
<td>-0.000112</td>
<td>( (462) ) 0.428 (797) 0.000032 (60)</td>
</tr>
<tr>
<td>32768</td>
<td>0.221300</td>
<td>-0.001928</td>
<td>( (825) ) -3.619 (2949) -0.000074 (55)</td>
</tr>
<tr>
<td>65536</td>
<td>0.221350</td>
<td>-0.000394</td>
<td>( (634) ) -5.272 (2827) -0.000087 (53)</td>
</tr>
<tr>
<td>131072</td>
<td>0.221390</td>
<td>0.000041</td>
<td>( (54) ) 1.231 (4779) 0.000015 (60)</td>
</tr>
<tr>
<td>262144</td>
<td>0.221390</td>
<td>0.000645</td>
<td>( (627) ) 2.640 (2821) 0.000033 (36)</td>
</tr>
<tr>
<td>524288</td>
<td>0.221400</td>
<td>-0.000615</td>
<td>( (430) ) -4.693 (2324) -0.000058 (31)</td>
</tr>
<tr>
<td>1048576</td>
<td>0.221420</td>
<td>0.001573</td>
<td>( (766) ) 7.370 (4820) 0.000082 (53)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L</th>
<th>( \xi_L )</th>
<th>m_L</th>
<th>( \partial m_L / \partial K_{nn} )</th>
<th>( \partial m_L / \partial \xi(t.o.u..) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.55</td>
<td>0.000000</td>
<td>( (73) ) -0.014 (17) -0.000755 (18145)</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.10</td>
<td>0.000040</td>
<td>( (234) ) -0.001 (20) -0.000007 (580)</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>2.20</td>
<td>-0.000014</td>
<td>( (124) ) 0.013 (32) -0.001022 (1072)</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>4.40</td>
<td>-0.000047</td>
<td>( (467) ) -0.195 (132) -0.005278 (12540)</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>8.80</td>
<td>0.000280</td>
<td>( (232) ) -1.491 (855) -0.002982 (1670)</td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>17.60</td>
<td>-0.000252</td>
<td>( (160) ) -3.619 (3029) 0.000315 (105)</td>
<td></td>
</tr>
<tr>
<td>128</td>
<td>35.20</td>
<td>0.000160</td>
<td>( (160) ) -3.619 (3029) 0.000315 (105)</td>
<td></td>
</tr>
</tbody>
</table>

Table (2.3): Raw and interpolated magnetisation per spin
<table>
<thead>
<tr>
<th>L</th>
<th>$\beta$</th>
<th>$s_{nnL}$</th>
<th>$\partial s_{nn,L}/\partial K_{nn}$</th>
<th>$\partial s_{nn,L}/\partial \xi(t,0,u)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.089391</td>
<td>0.660089</td>
<td>0.0338 (9) 0.516168 (18655)</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>0.730890 (803)</td>
<td>0.0337 (5) 0.524624 (9590)</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.190000</td>
<td>0.698041 (229)</td>
<td>0.0983 (14) 0.187928 (8572)</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.150000</td>
<td>0.891473 (114)</td>
<td>0.7944 (97) 0.033676 (928)</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>0.219400</td>
<td>0.944920 (93)</td>
<td>4.4119 (360) 0.007805 (177)</td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>0.220880</td>
<td>0.970070 (179)</td>
<td>23.1311 (4831) 0.001857 (225)</td>
<td></td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>0.972025 (52)</td>
<td>85.3050 (4085) 0.001752 (223)</td>
<td></td>
</tr>
<tr>
<td>256</td>
<td>0.221500</td>
<td>0.980626 (29)</td>
<td>86.3065 (3728) 0.001421 (97)</td>
<td></td>
</tr>
<tr>
<td>512</td>
<td>0.221800</td>
<td>0.981722 (25)</td>
<td>88.0487 (4246) 0.001112 (44)</td>
<td></td>
</tr>
<tr>
<td>1024</td>
<td>0.221900</td>
<td>0.982536 (21)</td>
<td>88.9524 (2144) 0.001106 (29)</td>
<td></td>
</tr>
</tbody>
</table>

Table (2.4): The raw and interpolated nearest neighbour interaction per spin.
The nearest neighbour interaction per spin.

Figure (2.4) The nearest neighbour interaction per spin.
<table>
<thead>
<tr>
<th>L</th>
<th>$\beta$</th>
<th>$S_L^2$</th>
<th>$\partial S_L^2/\partial \kappa_{nn}$</th>
<th>$\partial S_L^2/\partial \xi(2\pi/L;0,0,0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.089391</td>
<td>0.9</td>
<td>0.0 (1)</td>
<td>0.0 (1)</td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>1.9 (1)</td>
<td>0.0 (1)</td>
<td>0.0 (1)</td>
</tr>
<tr>
<td>8</td>
<td>0.190000</td>
<td>5.0 (1)</td>
<td>1.0 (1)</td>
<td>1.9 (2)</td>
</tr>
<tr>
<td></td>
<td>0.200000</td>
<td>5.6 (1)</td>
<td>0.9 (1)</td>
<td>1.0 (1)</td>
</tr>
<tr>
<td></td>
<td>0.205000</td>
<td>5.9 (1)</td>
<td>0.8 (1)</td>
<td>0.6 (1)</td>
</tr>
<tr>
<td></td>
<td>0.210000</td>
<td>6.0 (1)</td>
<td>0.3 (1)</td>
<td>0.2 (1)</td>
</tr>
<tr>
<td></td>
<td>0.211000</td>
<td>6.1 (1)</td>
<td>0.1 (1)</td>
<td>0.0 (1)</td>
</tr>
<tr>
<td>16</td>
<td>0.215000</td>
<td>19.0 (27)</td>
<td>39.2 (65)</td>
<td>1.7 (3)</td>
</tr>
<tr>
<td></td>
<td>0.215200</td>
<td>20.6 (1)</td>
<td>42.9 (6)</td>
<td>1.8 (1)</td>
</tr>
<tr>
<td></td>
<td>0.215500</td>
<td>20.8 (1)</td>
<td>42.3 (28)</td>
<td>1.6 (1)</td>
</tr>
<tr>
<td>32</td>
<td>0.219400</td>
<td>77.9 (3)</td>
<td>2033.5 (595)</td>
<td>3.6 (2)</td>
</tr>
<tr>
<td></td>
<td>0.219420</td>
<td>77.8 (3)</td>
<td>2101.9 (502)</td>
<td>3.8 (1)</td>
</tr>
<tr>
<td></td>
<td>0.219450</td>
<td>78.1 (1)</td>
<td>1964.2 (445)</td>
<td>3.4 (1)</td>
</tr>
<tr>
<td>64</td>
<td>0.220880</td>
<td>297.4 (42)</td>
<td>98737.5 (85977)</td>
<td>7.9 (18)</td>
</tr>
<tr>
<td></td>
<td>0.220890</td>
<td>298.5 (7)</td>
<td>96208.6 (20929)</td>
<td>7.3 (3)</td>
</tr>
<tr>
<td></td>
<td>0.220896</td>
<td>299.3 (5)</td>
<td>95828.1 (9075)</td>
<td>7.3 (1)</td>
</tr>
<tr>
<td></td>
<td>0.220899</td>
<td>300.2 (6)</td>
<td>95778.1 (16599)</td>
<td>7.3 (3)</td>
</tr>
<tr>
<td></td>
<td>0.220902</td>
<td>300.1 (6)</td>
<td>93888.3 (14117)</td>
<td>7.0 (2)</td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>1043.3 (76)</td>
<td>1132375.0 (1249750)</td>
<td>23.3 (54)</td>
</tr>
<tr>
<td></td>
<td>0.221350</td>
<td>1103.8 (52)</td>
<td>1234278.0 (693734)</td>
<td>20.3 (24)</td>
</tr>
<tr>
<td></td>
<td>0.221390</td>
<td>1163.8 (78)</td>
<td>1131337.0 (641186)</td>
<td>14.1 (17)</td>
</tr>
<tr>
<td></td>
<td>0.221390</td>
<td>1136.8 (55)</td>
<td>1060244.0 (397771)</td>
<td>13.4 (10)</td>
</tr>
<tr>
<td></td>
<td>0.221400</td>
<td>1159.1 (40)</td>
<td>1129574.0 (290886)</td>
<td>14.0 (7)</td>
</tr>
<tr>
<td></td>
<td>0.221420</td>
<td>1170.3 (68)</td>
<td>1117311.0 (681678)</td>
<td>12.4 (12)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L</th>
<th>$\xi_L$</th>
<th>$S_L^2$</th>
<th>$\partial S_L^2/\partial \kappa_{nn}$</th>
<th>$\partial S_L^2/\partial \xi(2\pi/L;0,0,0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.55</td>
<td>0.9</td>
<td>0.0 (1)</td>
<td>0.3 (4)</td>
</tr>
<tr>
<td>4</td>
<td>1.10</td>
<td>1.94 (1)</td>
<td>0.6 (1)</td>
<td>0.8 (1)</td>
</tr>
<tr>
<td>8</td>
<td>2.20</td>
<td>5.83 (1)</td>
<td>44.6 (5)</td>
<td>0.7 (3)</td>
</tr>
<tr>
<td>16</td>
<td>4.40</td>
<td>20.69 (2)</td>
<td>1972.2 (127)</td>
<td>1.2 (51)</td>
</tr>
<tr>
<td>32</td>
<td>8.80</td>
<td>78.55 (54)</td>
<td>95122.7 (7962)</td>
<td>3.5 (40)</td>
</tr>
<tr>
<td>64</td>
<td>17.60</td>
<td>299.38 (37)</td>
<td>1132910.1 (203414)</td>
<td>15.0 (28)</td>
</tr>
</tbody>
</table>

Table (2.5): Raw and interpolated estimates for $<S^2>$
Figure (2.5): The modulus squared Fourier transform of the magnetisation per spin interpolated to $t^*$ versus $L$.

$S^2(2\pi/L; t^*, 0, u^*) \nu L$

$\text{Wall.. } \gamma/\nu=1.959(5)$
<table>
<thead>
<tr>
<th>L</th>
<th>β</th>
<th>$x_L$</th>
<th>$\partial x_L / \partial k_{nn}$</th>
<th>$\partial x_L / \partial \xi(t,0,u..)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.083931</td>
<td>3.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>7.7 (1)</td>
<td>0.7 (1)</td>
<td>10.3 (3)</td>
</tr>
<tr>
<td>8</td>
<td>0.181700</td>
<td>7.7 (1)</td>
<td>0.7 (1)</td>
<td>10.5 (1)</td>
</tr>
<tr>
<td>16</td>
<td>0.190000</td>
<td>11.8 (1)</td>
<td>7.2 (3)</td>
<td>13.7 (5)</td>
</tr>
<tr>
<td>32</td>
<td>0.200000</td>
<td>18.5 (1)</td>
<td>14.8 (5)</td>
<td>16.5 (5)</td>
</tr>
<tr>
<td>64</td>
<td>0.205000</td>
<td>24.6 (2)</td>
<td>23.2 (8)</td>
<td>19.1 (5)</td>
</tr>
<tr>
<td>128</td>
<td>0.210000</td>
<td>34.3 (1)</td>
<td>39.2 (11)</td>
<td>21.5 (4)</td>
</tr>
<tr>
<td>256</td>
<td>0.211000</td>
<td>36.9 (1)</td>
<td>41.8 (14)</td>
<td>21.6 (1)</td>
</tr>
<tr>
<td>512</td>
<td>0.215000</td>
<td>73.4 (6)</td>
<td>747.2 (171)</td>
<td>31.7 (7)</td>
</tr>
<tr>
<td>1024</td>
<td>0.215200</td>
<td>82.6 (2)</td>
<td>850.0 (116)</td>
<td>35.2 (3)</td>
</tr>
<tr>
<td>2048</td>
<td>0.215500</td>
<td>86.6 (4)</td>
<td>926.7 (185)</td>
<td>35.9 (7)</td>
</tr>
<tr>
<td>32768</td>
<td>0.219400</td>
<td>305.1 (27)</td>
<td>37494.3 (6848)</td>
<td>66.3 (11)</td>
</tr>
<tr>
<td>65536</td>
<td>0.219420</td>
<td>310.8 (11)</td>
<td>37584.4 (2707)</td>
<td>68.1 (8)</td>
</tr>
<tr>
<td>131072</td>
<td>0.219450</td>
<td>312.4 (11)</td>
<td>38243.3 (3086)</td>
<td>66.9 (6)</td>
</tr>
<tr>
<td>262144</td>
<td>0.220880</td>
<td>1154.8 (72)</td>
<td>1618336.2 (172306)</td>
<td>129.9 (19)</td>
</tr>
<tr>
<td>524288</td>
<td>0.220890</td>
<td>1182.3 (83)</td>
<td>1706172.6 (254146)</td>
<td>129.8 (16)</td>
</tr>
<tr>
<td>1048576</td>
<td>0.220896</td>
<td>1191.8 (39)</td>
<td>1713254.6 (107329)</td>
<td>130.6 (8)</td>
</tr>
<tr>
<td>2097152</td>
<td>0.220899</td>
<td>1189.2 (79)</td>
<td>1702468.9 (235314)</td>
<td>130.5 (15)</td>
</tr>
<tr>
<td>4194304</td>
<td>0.220902</td>
<td>1198.7 (52)</td>
<td>1747359.1 (158717)</td>
<td>129.8 (10)</td>
</tr>
<tr>
<td>8388608</td>
<td>0.221300</td>
<td>3054.8 (570)</td>
<td>10241810.8 (5187582)</td>
<td>210.3 (190)</td>
</tr>
<tr>
<td>16777216</td>
<td>0.221350</td>
<td>3906.1 (555)</td>
<td>14855290.0 (4541545)</td>
<td>244.6 (99)</td>
</tr>
<tr>
<td>33554432</td>
<td>0.221390</td>
<td>4484.1 (947)</td>
<td>19831353.4 (7239364)</td>
<td>247.4 (93)</td>
</tr>
<tr>
<td>67108864</td>
<td>0.221390</td>
<td>4521.1 (419)</td>
<td>19461375.8 (4000204)</td>
<td>245.8 (53)</td>
</tr>
<tr>
<td>134217728</td>
<td>0.221400</td>
<td>4720.9 (315)</td>
<td>20644112.3 (2913930)</td>
<td>256.7 (37)</td>
</tr>
<tr>
<td>268435456</td>
<td>0.221420</td>
<td>5079.6 (686)</td>
<td>23713264.0 (6317416)</td>
<td>264.0 (75)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L</th>
<th>$\xi_L$</th>
<th>$x_L$</th>
<th>$\partial x_L / \partial k_{nn}$</th>
<th>$\partial x_L / \partial \xi(t,0,u..)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.55</td>
<td>3.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1.10</td>
<td>7.7 (1)</td>
<td>0.69 (1)</td>
<td>9.9 (35)</td>
</tr>
<tr>
<td>8</td>
<td>2.20</td>
<td>23.1 (1)</td>
<td>23.21 (37)</td>
<td>18.3 (1)</td>
</tr>
<tr>
<td>16</td>
<td>4.40</td>
<td>82.2 (2)</td>
<td>851.52 (368)</td>
<td>31.0 (23)</td>
</tr>
<tr>
<td>32</td>
<td>8.80</td>
<td>310.6 (19)</td>
<td>37758.0 (28266)</td>
<td>61.6 (650)</td>
</tr>
<tr>
<td>64</td>
<td>17.60</td>
<td>1192.5 (73)</td>
<td>1724968.20 (1230062)</td>
<td>104.9 (385)</td>
</tr>
<tr>
<td>128</td>
<td>35.20</td>
<td>4580.0 (522)</td>
<td>19941782.42 (22156294)</td>
<td>239.2 (1285)</td>
</tr>
</tbody>
</table>

Table (2.6): The raw and interpolated susceptibility per spin.
Figure (2.6): The susceptibility per spin.

\[ \chi(t^*, 0, u^*) \propto L \]

Wall.. $\gamma/\nu = 1.959(5)$
Table (2.7): The raw and interpolated 4th magnetic cumulant per spin.

<table>
<thead>
<tr>
<th>L</th>
<th>$\chi_L^{(4)}$</th>
<th>$-\partial \chi_L^{(4)}/\partial K_{nn}(t,0,u,..)$</th>
<th>$\partial \chi_L^{(4)}/\partial \xi(t,0,u,..)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.089391</td>
<td>0.126 $10^3$</td>
<td>0.34 $10^2$</td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>0.260 $10^4$ (0.23 $10^2$)</td>
<td>0.701 $10^3$ (0.34 $10^2$)</td>
</tr>
<tr>
<td></td>
<td>0.181700</td>
<td>0.270 $10^4$ (0.58 $10^1$)</td>
<td>0.722 $10^3$ (0.19 $10^2$)</td>
</tr>
<tr>
<td>8</td>
<td>0.190000</td>
<td>0.159 $10^5$ (0.13 $10^3$)</td>
<td>0.314 $10^5$ (0.79 $10^4$)</td>
</tr>
<tr>
<td></td>
<td>0.200000</td>
<td>0.694 $10^5$ (0.23 $10^3$)</td>
<td>0.175 $10^5$ (0.41 $10^4$)</td>
</tr>
<tr>
<td></td>
<td>0.205000</td>
<td>0.170 $10^6$ (0.55 $10^4$)</td>
<td>0.490 $10^6$ (0.40 $10^5$)</td>
</tr>
<tr>
<td></td>
<td>0.210000</td>
<td>0.461 $10^6$ (0.43 $10^4$)</td>
<td>0.153 $10^7$ (0.70 $10^5$)</td>
</tr>
<tr>
<td></td>
<td>0.211000</td>
<td>0.567 $10^6$ (0.54 $10^4$)</td>
<td>0.188 $10^7$ (0.88 $10^5$)</td>
</tr>
<tr>
<td>16</td>
<td>0.215000</td>
<td>0.487 $10^7$ (0.40 $10^5$)</td>
<td>0.221 $10^9$ (0.98 $10^6$)</td>
</tr>
<tr>
<td></td>
<td>0.215200</td>
<td>0.127 $10^8$ (0.94 $10^5$)</td>
<td>0.412 $10^9$ (0.69 $10^7$)</td>
</tr>
<tr>
<td></td>
<td>0.215500</td>
<td>0.149 $10^8$ (0.24 $10^6$)</td>
<td>0.496 $10^9$ (0.16 $10^8$)</td>
</tr>
<tr>
<td></td>
<td>0.219400</td>
<td>0.129 $10^10$ (0.57 $10^8$)</td>
<td>0.513 $10^{12}$ (0.30 $10^{11}$)</td>
</tr>
<tr>
<td></td>
<td>0.219420</td>
<td>0.134 $10^10$ (0.42 $10^8$)</td>
<td>0.505 $10^{12}$ (0.17 $10^{11}$)</td>
</tr>
<tr>
<td></td>
<td>0.219450</td>
<td>0.133 $10^10$ (0.27 $10^8$)</td>
<td>0.513 $10^{12}$ (0.11 $10^{11}$)</td>
</tr>
<tr>
<td>64</td>
<td>0.220880</td>
<td>0.142 $10^{12}$ (0.27 $10^{11}$)</td>
<td>0.601 $10^{15}$ (0.13 $10^{15}$)</td>
</tr>
<tr>
<td></td>
<td>0.220890</td>
<td>0.150 $10^{12}$ (0.46 $10^{11}$)</td>
<td>0.694 $10^{15}$ (0.25 $10^{14}$)</td>
</tr>
<tr>
<td></td>
<td>0.220896</td>
<td>0.157 $10^{12}$ (0.26 $10^{11}$)</td>
<td>0.708 $10^{15}$ (0.11 $10^{14}$)</td>
</tr>
<tr>
<td></td>
<td>0.220899</td>
<td>0.154 $10^{12}$ (0.40 $10^{11}$)</td>
<td>0.691 $10^{15}$ (0.22 $10^{14}$)</td>
</tr>
<tr>
<td></td>
<td>0.220902</td>
<td>0.154 $10^{12}$ (0.34 $10^{11}$)</td>
<td>0.717 $10^{15}$ (0.15 $10^{14}$)</td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>0.393 $10^{13}$ (0.56 $10^{12}$)</td>
<td>0.392 $10^{17}$ (0.63 $10^{16}$)</td>
</tr>
<tr>
<td></td>
<td>0.221350</td>
<td>0.116 $10^{14}$ (0.62 $10^{12}$)</td>
<td>0.140 $10^{18}$ (0.78 $10^{16}$)</td>
</tr>
<tr>
<td></td>
<td>0.221390</td>
<td>0.143 $10^{14}$ (0.17 $10^{13}$)</td>
<td>0.207 $10^{18}$ (0.23 $10^{17}$)</td>
</tr>
<tr>
<td></td>
<td>0.221390</td>
<td>0.169 $10^{14}$ (0.71 $10^{12}$)</td>
<td>0.233 $10^{18}$ (0.68 $10^{16}$)</td>
</tr>
<tr>
<td></td>
<td>0.221400</td>
<td>0.198 $10^{14}$ (0.81 $10^{12}$)</td>
<td>0.272 $10^{18}$ (0.97 $10^{16}$)</td>
</tr>
<tr>
<td></td>
<td>0.221420</td>
<td>0.228 $10^{14}$ (0.18 $10^{13}$)</td>
<td>0.335 $10^{18}$ (0.25 $10^{17}$)</td>
</tr>
</tbody>
</table>

-72-
Figure (2.7): The fourth magnetic cumulant per spin.
<table>
<thead>
<tr>
<th>( L )</th>
<th>( \beta )</th>
<th>( \xi_L )</th>
<th>( \partial \xi_L / \partial K_{nn}(t,0,u^*) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.089391</td>
<td>0.55</td>
<td>(1)</td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>1.09</td>
<td>(1)</td>
</tr>
<tr>
<td>8</td>
<td>0.190000</td>
<td>1.10</td>
<td>(1)</td>
</tr>
<tr>
<td>16</td>
<td>0.210000</td>
<td>1.49</td>
<td>(1)</td>
</tr>
<tr>
<td>32</td>
<td>0.219400</td>
<td>1.93</td>
<td>(1)</td>
</tr>
<tr>
<td>64</td>
<td>0.220880</td>
<td>2.27</td>
<td>(1)</td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>2.75</td>
<td>(1)</td>
</tr>
<tr>
<td>128</td>
<td>0.221400</td>
<td>2.88</td>
<td>(1)</td>
</tr>
<tr>
<td>64</td>
<td>0.220902</td>
<td>4.31</td>
<td>(2)</td>
</tr>
<tr>
<td>32</td>
<td>0.219450</td>
<td>4.41</td>
<td>(2)</td>
</tr>
<tr>
<td>16</td>
<td>0.215200</td>
<td>4.53</td>
<td>(2)</td>
</tr>
<tr>
<td>8</td>
<td>0.219420</td>
<td>8.70</td>
<td>(7)</td>
</tr>
<tr>
<td>16</td>
<td>0.219420</td>
<td>8.81</td>
<td>(4)</td>
</tr>
<tr>
<td>32</td>
<td>0.219450</td>
<td>8.82</td>
<td>(2)</td>
</tr>
<tr>
<td>64</td>
<td>0.220899</td>
<td>17.29</td>
<td>(56)</td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>17.53</td>
<td>(8)</td>
</tr>
<tr>
<td>64</td>
<td>0.220896</td>
<td>17.59</td>
<td>(5)</td>
</tr>
<tr>
<td>32</td>
<td>0.220899</td>
<td>17.53</td>
<td>(9)</td>
</tr>
<tr>
<td>16</td>
<td>0.220902</td>
<td>17.63</td>
<td>(6)</td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>28.29</td>
<td>(34)</td>
</tr>
<tr>
<td>64</td>
<td>0.221350</td>
<td>32.46</td>
<td>(38)</td>
</tr>
<tr>
<td>32</td>
<td>0.221390</td>
<td>34.41</td>
<td>(59)</td>
</tr>
<tr>
<td>16</td>
<td>0.221390</td>
<td>35.15</td>
<td>(27)</td>
</tr>
<tr>
<td>64</td>
<td>0.221400</td>
<td>35.71</td>
<td>(18)</td>
</tr>
<tr>
<td>128</td>
<td>0.221420</td>
<td>37.23</td>
<td>(38)</td>
</tr>
</tbody>
</table>

Table (2.8): The correlation length and the temperature, raw and interpolated.
Figure (2.8) The interpolation temperature $\beta^*$ minus the estimate $0.221654(5)$ for $K_{nn,c}$ of Pawley et al (1984).
<table>
<thead>
<tr>
<th>L</th>
<th>β</th>
<th>-g&lt;sub&gt;RL&lt;/sub&gt;</th>
<th>-∂g&lt;sub&gt;RL&lt;/sub&gt;/∂K&lt;sub&gt;nn&lt;/sub&gt;</th>
<th>-∂g&lt;sub&gt;RL&lt;/sub&gt;/∂ξ(t,0,u..)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.089391</td>
<td>61.72</td>
<td>(1)</td>
<td>66.97</td>
</tr>
<tr>
<td>4</td>
<td>0.181200</td>
<td>33.89</td>
<td>(37)</td>
<td>-2.94</td>
</tr>
<tr>
<td>8</td>
<td>0.190000</td>
<td>29.07</td>
<td>(22)</td>
<td>-9.68</td>
</tr>
<tr>
<td>16</td>
<td>0.210000</td>
<td>18.78</td>
<td>(11)</td>
<td>-18.03</td>
</tr>
<tr>
<td>32</td>
<td>0.219400</td>
<td>20.98</td>
<td>(57)</td>
<td>-80.62</td>
</tr>
<tr>
<td>64</td>
<td>0.219450</td>
<td>19.86</td>
<td>(26)</td>
<td>-1073.20</td>
</tr>
<tr>
<td>128</td>
<td>0.221300</td>
<td>18.62</td>
<td>(176)</td>
<td>-35391.01</td>
</tr>
<tr>
<td>2</td>
<td>0.55</td>
<td>61.72</td>
<td>(1)</td>
<td>66.97</td>
</tr>
<tr>
<td>4</td>
<td>1.10</td>
<td>33.69</td>
<td>(9)</td>
<td>-2.49</td>
</tr>
<tr>
<td>8</td>
<td>2.20</td>
<td>24.73</td>
<td>(22)</td>
<td>-9.68</td>
</tr>
<tr>
<td>16</td>
<td>4.40</td>
<td>26.87</td>
<td>(22)</td>
<td>-101.90</td>
</tr>
<tr>
<td>32</td>
<td>8.80</td>
<td>21.65</td>
<td>(26)</td>
<td>-675.86</td>
</tr>
<tr>
<td>64</td>
<td>17.60</td>
<td>20.25</td>
<td>(35)</td>
<td>-14728.31</td>
</tr>
<tr>
<td>128</td>
<td>35.20</td>
<td>19.64</td>
<td>(44)</td>
<td>-35391.40</td>
</tr>
</tbody>
</table>

Table (2.9): The raw and interpolated renormalised coupling per spin.
Figure (2.9) The renormalised coupling constant
The quantitative measure of hyperscaling and values for exponents must be extracted from the interpolated results tabulated and shown graphically above. Taking the log of the various interpolated quantities and plotting versus \( \log L \) gives a curve which tends to a straight line as \( L \) becomes large and the corrections to scaling become small. Below in table (2.10) the straight line slopes joining points on lattice sizes differing by a factor of 2 are indicated. Reading each row from right to left the exponents seem to be converging to some limit as the two lattices compared become large. The straight line slope joining points from lattices differing by a factor of 4 and then 8 are also given.

<table>
<thead>
<tr>
<th>exponent</th>
<th>( L^{128v64} )</th>
<th>( L^{64v32} )</th>
<th>( L^{32v16} )</th>
<th>( L^{16v8} )</th>
<th>( L^{8v4} )</th>
<th>( L^{4v2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1-\alpha)\nu)</td>
<td>1.472</td>
<td>1.285</td>
<td>1.223</td>
<td>1.133</td>
<td>0.923</td>
<td>0.574</td>
</tr>
<tr>
<td>(\gamma/\nu)</td>
<td>1.939</td>
<td>1.931</td>
<td>1.925</td>
<td>1.827</td>
<td>1.587</td>
<td>1.108</td>
</tr>
<tr>
<td>(\gamma/\nu)</td>
<td>1.942</td>
<td>1.941</td>
<td>1.918</td>
<td>1.832</td>
<td>1.585</td>
<td>1.138</td>
</tr>
<tr>
<td>((\gamma+2\Delta)\nu)</td>
<td>6.927</td>
<td>6.898</td>
<td>6.701</td>
<td>6.352</td>
<td>5.841</td>
<td>4.401</td>
</tr>
<tr>
<td>(1/\nu)</td>
<td>1.5697</td>
<td>1.5619</td>
<td>1.5330</td>
<td>1.4149</td>
<td>1.2234</td>
<td></td>
</tr>
<tr>
<td>(w)</td>
<td>0.055</td>
<td>0.016</td>
<td>0.137</td>
<td>0.305</td>
<td>0.494</td>
<td>0.875</td>
</tr>
</tbody>
</table>

\[ w\left(\frac{L}{128}\right)^{128v32} = 0.019 \]
\[ w\left(\frac{L}{64}\right)^{64v16} = 0.060 \]
\[ w\left(\frac{L}{32}\right)^{32v8} = 0.2217 \]
\[ w\left(\frac{L}{16}\right)^{16v4} = 0.1422 \]

**Table (2.10):** Exponent trends from slope of log plot versus \( \log L \).

The exponents in table (2.10) appear to tend to an asymptotic limit as the two lattices compared become large and the effect of corrections to scaling is reduced. This trend also indicates, as did two parameters fits, that a correction to scaling needs to be included in the fitting for lattices smaller than \( L=16 \).

A fit with 4 parameters

\[ y=AL^c(1+BL^b) \quad (2.30) \]

plus an additive constant for the specific heat and the nearest neighbour
interaction the only constraint being that b is less than 0, i.e. a correction to scaling, gives the following estimates. Only lattices greater than L=4 are included in this fit so that the chi-squared corresponds to 2 free parameters (1 free parameter for $S_{nn}$ and $C_h$).

<table>
<thead>
<tr>
<th>$A$</th>
<th>$a$</th>
<th>$B$</th>
<th>$b$</th>
<th>$C$</th>
<th>$X^2_{[f=2]}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{\nu}$</td>
<td>0.5629(74)</td>
<td>$-1.584(5)$</td>
<td>$-1.38(4)$</td>
<td>$-0.974(10)$</td>
<td>1.41</td>
</tr>
<tr>
<td>$\frac{\gamma}{\nu}$</td>
<td>0.0896(2)</td>
<td>1.959(3)</td>
<td>5.38(3)</td>
<td>$-1.79(5)$</td>
<td>2.8</td>
</tr>
<tr>
<td>$(\gamma+2\Delta)/\nu$</td>
<td>$-4.996(5)$</td>
<td>6.921(29)</td>
<td>35.1(19)</td>
<td>$-1.81(8)$</td>
<td>2.3</td>
</tr>
<tr>
<td>$w'$</td>
<td>$-20.4(17)$</td>
<td>$-0.008(20)$</td>
<td>5.4(6)</td>
<td>$-1.51(13)$</td>
<td>2.4</td>
</tr>
</tbody>
</table>

Table (2.10): 4 parameter fit to $L=8, 16, 32, 64, 128$ interpolated data.

A very similar set of exponent values was obtained including only the $L=8, L=16, L=32, L=64$ and $L=128$ corresponding to $f=1$ for fits with 4 parameters.

| $1/\nu=1.580(5)$ | $\chi^2=1.41$ |
| $\frac{\gamma}{\nu}=1.956(6)$ | $\chi^2=1.32$ |
| $(\gamma+2\Delta)/\nu=6.918(19)$ | $\chi^2=2.03$ |
| $w'=0.0003(202)$ | $\chi^2=1.6$ |

Increasing the errors in the exponent estimates of table (2.10) so that they correspond to confidence levels of 67% gives:

$\frac{\gamma}{\nu}=1.959(5); (\gamma+2\Delta)/\nu=6.921(34)$
\[ 1/\nu = 1.584(4); \ w^* = 0.008(24) \]

These correspond to

\[ \nu = 0.631(2); \ \gamma = 1.236(4); \ \Delta = 1.568(8); \ w^* = 0.008(24) \]

which we compare with the estimates of Fisher and Chen (1985):

\[ \nu = 0.632(1); \ \gamma = 1.2395(4); \ \alpha = 0.105(7) \]

which imply,

\[ w^* = 0.0016(160), \ \Delta = 1.5672(8). \]

Using the definition \[ w^* = \nu - (2\Delta - \gamma) \] a consistency check for \( w^* \) calculated by substituting our estimates for \( \nu, \gamma, \Delta \) gives \[ w^* = 0.007(26). \]

2.6. Conclusions

We conclude that our estimate for \( w^* = 0.008(24) \) adds MC support to the validity of hyperscaling in the three dimensional Ising model. The finite size scaling analysis has also given estimates for \( \nu, \gamma, \Delta \) in good agreement with Fisher and Chen (1985). Providing we can obtain a reasonable estimate for \( \alpha \) then the accord of exponent estimates obtained with those obtained by other methods can be taken as an \textit{a posteriori} measure of the validity of the finite size scaling analysis applied. With these provisos the estimate for Fisher's anomalous exponent is then taken as a measure of the validity of hyperscaling in the model which we have been able to see by brute force simulation of large lattices.
Critical comparison of results with those of Freedman and Baker

There are some discrepancies between the results we have obtained, embodied in tables and graphs (2.3) to (2.9) inclusive, and those obtained by Freedman and Baker (1982). Our results for $K_{nn}^*$ for various system sizes are in agreement within errors with those of Freedman and Baker which implies agreement for the correlation length estimates. However figure (2.9) shows a systematic discrepancy of several standard deviations with Freedman and Baker for estimates of the renormalised coupling, $g_R$, for lattices of $L=8$ to $L=64$.

One possible cause for this systematic discrepancy could be that the estimates for $g_R$ come from a set of correlated configurations. This would have 2 effects. The first is a systematic shift in $g_R$ as suggested to me by Dr. A. D. Bruce using the following argument. Suppose that somehow only one configuration is used, because of say poverty in the random generator, so that configurations are never changed during the entire simulation. In this case $g_{R,L}(K_{nn}^*)$ is $-2.1/c^3 = -96.168$. So $g_R$ will tend to be closer to $-96.168$ than it should be if the totality of data used to find the best estimate is correlated. If Freedman and Baker's data somehow suffers from this problem then it is possible that corrective action would bring their data into agreement with ours. If our data suffers from this disease then the discrepancy will be increased since corrected data moves towards increasing $g_R$, i.e. down page 77. The other by product of correlated configurations is under estimated errors. Corrective action involves increasing the errorbars. We require an increase in errorbars of a factor of $\sim 5$ before our results can be reconciled with those of Freedman and Baker.

Is there any evidence for under estimated errorbars and/or correlations between configurations over MC time scales exceeding what we have taken to be the minimum independent bin size ($\sim 1000,000$ MCS/spin for $L=128$) or worse still exceeding the total number of MC steps for a particular size and $K_{nn}$ value?

For $L=2...64$ the uncertainty assignments seem to be sensible. The uncertainty assignments for $L=128$, however, are under estimated as is particularly obvious for $g_{R,128}$. Having checked the binning procedure and confirmed the stability of error estimates for bins greater than 500,000 MCS/spin the only explanation we can offer is that g05fast (used only for
L=128) is giving rise to very long time correlations.

We have tested g05fast and seen it be trustworthy up to 300,000,000 calls. If we assume the worst, that g05fast repeats itself after 300,000,000 calls, then we should scale the uncertainty assignments for the L=128 data up by the factor sqrt(number of calls to g05fast/300,000,000). For lattices L=4,..64 a tried and tested random number generator g05xorreal (used by Pawley et al (1984)) was used so this data is not thought to suffer from such random number time correlation effects. The scaling factors for $K_{nn}=0.2213, 0.22135, 0.22139, 0.22139, 0.2214, 0.22142$ are respectively 1.0, 1.85, 2.27, 1.85, 3.33, and 1.69. The corresponding values for g_{R,128} are 18.62(1.72), 22.22(1.98), 17.47(2.7), 18.99(1.52), 19.54(1.77) and 17.14(1.03). Scaling all the L=128 uncertainty assignments in this way and interpolating to $\xi(K_{nn}^*)=cL$ modifies the L=128 point for each of the quantities used in the finite size scaling fits. The resulting quantities are:

\[
S_{nn,128}(K_{nn}^*) = 0.98182(6)
\]
\[
<S^2(K_{nn}^*)>_{128} = 1146.4(6.3)
\]
\[
\chi^{(2)}_{128}(K_{nn}^*) = 4568.6(59.5)
\]
\[
\chi^{(4)}_{128}(K_{nn}^*) = 1.733(93) \times 10^{13}
\]
\[
K_{nn,128}^* = 0.221393(3)
\]
\[
g_{R,128}(K_{nn}^*) = 19.38(85)
\]

From these results we see that the interpolated values are changed a small amount while the error has increased. The best estimates for exponents, obtained from a 4 parameter fit to the L=4, 8, 16, 32, 64 interpolated data of tables (2.2) to (2.9) and the new L=128 interpolated data, are:

\[
1/\nu=1.579(10)
\]
\[
\gamma/\nu=1.952(9)
\]
\[
(\gamma+2\Delta)/\nu=6.928(33)
\]
\[
w^* = 0.004(50)
\]

The errors again correspond to confidence levels of 67%. The above values
correspond to

\[ v=0.633(4); \ \gamma=1.236(14); \ \Delta=1.575(19); \ w^*=0.004(50) \]

Our conclusions on page 80 still hold since though our results are slightly modified they are still in agreement with the results quoted on page 80 to within our new more modest claims for errorbars.
3.1. Introduction

The test of hyperscaling described in chapter 2 illustrates the finite size scaling method of extracting bulk critical properties such as exponents and universal scaling functions from a Monte Carlo importance sampling simulation. The consistency of the results with hyperscaling provides support for the correlation length scaling hypothesis and the renormalisation group description of critical phenomena. It is with this background in mind that in this chapter a real space renormalisation group method of analysis is combined with a Monte Carlo simulation in a so called MCRG simulation. Here again the three dimensional Ising model, for which many methods have yielded estimates for the critical exponents, provides a bench mark against which the MCRG method can be compared.

S. K. Ma (1976) first suggested that a Monte Carlo simulation combined with a renormalisation group analysis might provide a good non-perturbative numerical method of studying physics, particularly well suited to critical phenomena. The pruning of degrees of freedom by the RG transformation is performed exactly by generating blockspin configurations from spin configurations. In applying the RG rule, $b^d$ spins are combined using some exact rule to determine an effective blockspin. In this way the number of spins is pruned and a new blockspin configuration holds the key large distance features of the unblocked configuration. Indeed the exact nature of the (local) RG transformation means that a knowledge of the effective couplings after blocking is contained implicitly in the configurations of blockspins. There are many choices of blocking rule here. For the Ising model on a d dimensional hypercubic lattice the blockspins are to belong to the same set $\sigma' \in \{+1,-1\}$ and the lattice is to be a d dimensional hypercube of size $L/b$. The repeated application of the same blocking rule produces a sequence of blocked configurations representative of the renormalised Hamiltonian implicit in them. Schematically the MCRG approach is illustrated in figure (3.1).
Figure (3.1): Schematic representation of the MCRG method.

The flow of Hamiltonians in coupling constant space is illustrated for a standard fixed point in figure (3.2).

Figure (3.2): The effective Hamiltonians represented as points in the space of all coupling constants. The renormalisation group generates a flow initially towards the fixed point, for small relevant eigenperturbations but eventually away.

The renormalised correlation length illustrates the way in which MCRG is well suited to systems at criticality. Suppose the MC simulation is performed at a reduced temperature $t = (T-T_c)/T_c$, and the correlation length (which could be measured during the simulation) is $\xi(t)$ in units of lattice spacing $a$, where $0<\xi<L$, because of the finiteness of the system. After renormalisation the lattice spacing becomes $a' = ba$. A key assumption is that the correlation length, in physical units is the same before and after the renormalisation transformation. In units of the appropriate lattice spacings this requires:
\[ \xi'(t') = b^{-1} \xi(t) \]  

(3.1)

since \( \xi'(t') \) is measured in units of \( a' = ba \) and \( \xi(t) \) in units of \( a \). From this equation the only fixed points are \( \xi(t) = \xi'(t') = 0 \) or \( \infty \). The former corresponds to the trivial fixed points \( T = 0 \) or \( T = \infty \). The latter corresponds to a system at criticality and asserts that only systems at criticality remain there as the transformation is applied. Small relevant eigenperturbations corresponding to \( \xi < \infty \) inevitably flow to smaller \( \xi \)'s and further from criticality.

Let us recall some of the basic equations from chapter 1. The correlation length diverges as:

\[ \xi(t) = A|t|^{-\nu}. \]  

(3.2)

The renormalisation of \( t \) to \( t' \) follows from that of the relevant scaling field:

\[ u'(t') = \lambda_t u_t = b'y_u(t) \]  

(3.3)

Close to criticality \( u_t \sim c_t t \), so that we identify

\[ \nu = 1/\gamma_t \]  

(3.4)

with \( \gamma_t = \ln_e \lambda_t/\ln_e b \). Thus the eigenvalues \( \lambda \) of the stability matrix \( \partial K^{n+1}/\partial K^n |_K \) give the critical exponents, and the eigenvectors give the directions in \( K \) space of the various scaling fields. It is the calculation of this matrix which allows exponents to be estimated from a MCRG simulation.

Estimating the coupling constant flow directly and computationally differentiating \( K^{n+1} \) with respect to \( K^n \) is very expensive numerically because simulations at many points in coupling constant space are required, several for each coupling constant. It is also wasteful because the statistical correlations between different quantities are not exploited. Here an approach due to Wilson and Swendsen (1980) is used.

Correlation functions implicitly contain information about coupling constant flow. Consider how much the operator type \( \alpha \) at the \( n+1 \) blocking level, \( <S_{\alpha^{n+1}}> \), changes if the couplings, \( K^n \), embedded in the \( \alpha^n \) blocked
configuration are changed a small amount. The chain rule gives:

\[ \frac{\partial}{\partial K_B^n} \frac{\partial S_{n \alpha}}{\partial K^n} = \sum \left( \frac{\partial S_{n \gamma}}{\partial K^{n+1}} \frac{\partial K^{n+1}}{\partial K_B^n} \right) \] (3.5)

which, if the derivatives of the correlation functions can be measured, affords a means of obtaining the matrix of derivatives, \( \frac{\partial K^{n+1}}{\partial K^n} = T \) (as in chapter 1), by inversion. Again better use is made of statistical correlations if numerically differentiating several different runs is replaced by calculating the formal derivative and measuring the so generated correlation functions. We wish then to evaluate:

\[ \frac{\partial}{\partial K_B^n} \frac{\partial S_{n \alpha}}{\partial K^n} = \] (3.6)

where

\[ Z = \sum_{\{ \delta \}} \exp(\sum K^n \delta S^n \delta) \] (3.7)

Using the definition of the renormalisation group transformation given by equation (1.21) in chapter 1 and using the identity that \( Z^{(n)} = Z^{(n-1)} \) to divide the l.h.s by \( Z^{(n)} \) and the r.h.s. by \( Z^{(n-1)} \) re-expresses the R.G transformation as:

\[ \exp(K^n \cdot S^n) / (\sum_{\{ \delta \}} \exp(K^n \cdot S^n)) = \sum_{\{ \delta^n \}} \exp(K^{n-1} \cdot S^{n-1}) / (\sum_{\{ \delta^{n-1} \}} \exp(K^{n-1} \cdot S^{n-1})) \] (3.8)

so removing the \( G^n \) type terms and making the denominators the partition function divided by the level constant \( g^n \). This equation can be used on the r.h.s of (3.6) to make explicit the dependence of the r.h.s., at first sight dependent only on \( K^n \) and \( L/b^n \), on earlier couplings and the RG transformation. In particular (3.6) can be expressed as:
\[ \frac{\partial < S^n_\alpha >}{\partial K^m_B} = \frac{\partial}{\partial K^m_B} \left( \sum_{\sigma_1} \ldots \sum_{\sigma_m} S^n_\alpha P(\sigma^n, \sigma^{n-1}) \right) \]

\[ \cdot P(\sigma^{m+1}, \sigma^m) \exp(K^m S^m)/Z \]  

(3.9)

Now \( P(\sigma^n, \sigma^{n-1}) \) is independent of \( K^n \) for all \( n \) so the derivative simply pulls down terms from the exponentials:

\[ \frac{\partial < S^n_\alpha >}{\partial K^m_B} = \sum_{\sigma_1} \ldots \sum_{\sigma_m} S^n_\alpha S^m_B \]

\[ P(\sigma^n, \sigma^{n-1}) \cdot P(\sigma^{m+1}, \sigma^m) \exp(K^m S^m)/Z \]

-disconnected piece  

(3.10)

Using equation (3.3) and the constraint:

\[ \sum_{\xi} P(\sigma^p, \sigma^{p-1}) = 1 \]  

(3.11)

the derivative becomes:

\[ \frac{\partial < S^n_\alpha >}{\partial K^m_B} = < S^n_\alpha S^m_B >_c \]  

(3.12)

These quantities are all measurable during a simulation. The combination:

\[ P(\sigma^n, \sigma^{n-1}) \cdot P(\sigma^{m+1}, \sigma^m) \exp(K^m S^m)/Z \]  

(3.13)

is the combined probability of obtaining configuration \( \sigma^n \) at the \( n^{th} \) level of blocking from a configuration \( \sigma^m \) at the \( m^{th} \) level of blocking itself produced with probability \( \exp(K^m S^m)/Z \). This formal derivative is a big advantage over measuring \( < S^n_\alpha(K^n) > \) and \( < S^m_\alpha(K^m) > \) for several points along each coupling axis and numerically differentiating with respect to \( K^n \) and \( K^m \). Equation (3.5) can be inverted to give, using an obvious matrix notation:
\[ \frac{\partial K^{n+1}}{\partial K^{n}} = (\frac{\partial S^{n+1}}{\partial K^{n+1}})^{-1}(\frac{\partial S^{n+1}}{\partial K^{n}}). \quad (3.14) \]

Hence the matrix of derivatives can be obtained, on inserting the expression for the formal derivatives, (3.12), from measurable correlation functions. The characteristic equation:

\[ |\frac{\partial K^{n+1}}{\partial K^{n-1}} - \lambda| = 0 \quad (3.15) \]

gives the eigenvalues and hence the critical exponents associated with the leading and successive order corrections to scaling. So measurement of correlation functions dependent on the \( n^{th} \) and \( m^{th} \) blocking level of a particular configuration allows the matrix of derivatives, \( \frac{\partial K^{n}}{\partial K^{m}} \), which describes the coupling constant flow, to be found by inversion of a matrix problem of type \( Ax = b \). Equations (3.15) and (3.14) along with (3.12) are the fundamental ones in the MCRG approach.

3.2. The standard simulation

For a chosen Hamiltonian configurations typical of the equilibrium physics are generated using a Monte Carlo algorithm such as that of Metropolis \textit{et al} (1953) on a lattice of linear dimension \( L \) and dimensionality \( d \). The relative cost of updating and measuring and the correlation of successive configurations are to be taken into account when deciding how many updates to make in between measurements. Typically computer time is split 50:50 between updating and measuring. The RG rule such as majority rule is used on any configuration chosen to be measured to produce a sequence of coarse-grained or blocked configurations. Majority rule says: split the lattice into \( d \) dimensional hypercubes each of \( b^d \) spins. Form the sums of the \( b \) site spins in the cell. If this sum exceeds \( b^d/2 \) the cell spin is +1, if the sum is less than \( b^d/2 \) the cell spin is -1. If the sum is \( b^d/2 \) exactly as can be the case for \( b \) even on a simple cubic lattice then a random number is used to determine the cell spin. On the sequence \( \{\sigma^0\}, \{\sigma^1\}, \ldots \{\sigma^n\} \) all the quantities of interest, \(<S^n>_0, <S^n>_1, \ldots <S^n>_m \), are calculated and the correlation between this blocked sequence of, \( \{\sigma^0\}, \ldots \{\sigma^n\} \), is exploited to cut down the noise. The maximum number of blocking or RG levels is governed by the size of the zeroth level system since we must have more than 1 spin for any interesting
measurements to be made which places the constraint on \( n, L^d/(b^d)^n > 1 \).

To control finite size effects the whole MCRG simulation can be repeated on the same system with the same \( H^0 = \mathbf{K}^0 \mathbf{S}^0 \) but a different linear dimension.

The totality of data affords the means of obtaining a better estimate of \( K_{nn,c} \) and the whole critical hypersurface. If simulations are made at several values of \( K_{nn} \) about the best estimate for \( K_{nn,c} \) then all the data can be linearly (or quadratically) interpolated to \( K_{nn,c} \) with error estimates combined. The effect which truncating the recursion relation has on the eigenvalues and the eigenvectors can be investigated by including progressively more of the \( T \) matrix where care is taken to order the couplings according to a hierarchy of importance in the leading eigenvectors. This ordering, following Swendsen, has been based on the number of spins in the corresponding operator, and within a set of \( n \) spin couplings the most local are deemed most important. Ideally the \( T \) matrix should be diagonalised using the eigenvectors then the effect of removing (setting to zero) least relevant eigenperturbations or scaling fields in these eigendirections should be noted by successively removing more and more such terms from the largest \( T \) matrix available for analysis. The trend as more correlation functions and hence more of the implicit couplings are included is noted plotting eigenvalues versus truncation parameter. Of course it is not adequate just to note that successively irrelevant couplings individually alter less and less the eigenvalues; the real question is what is the effect of neglecting an infinite of such terms? Recent papers by Murthy and Shankar (1985) and Gupta, Murthy and Shankar (1985), indicate a procedure which allows an estimate of this truncation error to be made.

In summary, the raw data in this scheme is a set of estimates for the expectation values \( <S^n_\alpha> \), \( <S^n_\alpha S^m_\beta> \) for various \( \alpha, \beta, m \) and \( n \) on a range of lattice sizes, for a small number of \( K_{nn} \) values in the neighbourhood of the nearest neighbour critical point.

A very good discussion of such a simulation is given in a paper by Pawley Wallace R.H. Swendsen and K.G. Wilson (1984). In this chapter we shall extend the analysis of their data in order to follow the coupling constant flow.

### 3.3. Estimating the critical nearest neighbour coupling and coupling constant flow.

Wilson (1982) has suggested a particularly neat method of estimating \( K_{nn,c} \) by explicitly cancelling finite size effects. Consider how correlation functions
of blocked spins depending on effective couplings, \( K^n \), embedded in the blocked spins \( \sigma^n \) and hence, via the RG transformation, on the original configuration, \( \sigma^0 \), and hence on the original couplings \( K^0 = (K_{nn}, 0, 0, 0...) \) generated by the MC algorithm acting on \( H^0 \). From now on \( <S^n(K^n)>_L \) or \( S \) means: evaluate the quantities \( S \) on the \((L/b)^d\) block spins, \( \sigma^n \), in which the effective couplings \( K^n \) are embedded, and then average over the sequence of such blockspin configurations generated by the MCRG simulation. For a system of linear dimension \( L \) simulated with Hamiltonian \( H^0 = K^0.S^0 \) correlation functions for some general point in coupling constant space, say \( K_c \) which may be in the critical hypersurface if we wish, can be expanded as a Taylor series about \( K^0 \). This yields a relation:

\[
<S^n(K^n((K^0+(K_c-K^0))))>_L = <S^n(K^0)>_L + \partial <S^n(K^n((K^0)))>_L/K^0(K_c-K^0) + ... \tag{3.16}
\]

for which quadratic and higher terms can be neglected for \((K_c-K^0)\) sufficiently small. Again what sufficiently small means should be checked by estimating the correction terms and noting the effect of including successive correction terms on the results. A smaller system blocked fewer times can have its correlation functions similarly Taylor expanded about the same point, \( K_c \), to give

\[
<S^m(K^m(K^0+(K_c-K^0))))>_s = <S^m(K^0)>_s + \partial <S^m(K^m(K^0)))>_s/K^0(K_c-K^0) + ... \tag{3.17}
\]

For values of \( m \) and \( n \) such that the large system blocked \( n \) times and the small system blocked \( m \) times give rise to the same size blocked systems, the finite size effects are the same for both and any differences can only be due to differences in effective couplings. For an initial system close to critical hypersurface the effective couplings \( K^n \) and \( K^m \) of (3.16) and (3.17) differ by an amount controlled by the magnitude of the scaling fields \( u^n \) and \( u^m \). Explicitly if we expand the left hand sides of (3.16) and (3.17) about the fixed point \( K^* \) assuming that \( u^n \) and \( u^m \) are small then we find:
\[
\frac{\langle S^n(K^n(K^0)) \rangle_L}{\langle S^m(K^m(K^0)) \rangle_s} = \frac{(K_c-K^0)\partial \langle S^m(K^m(K^0)) \rangle_s}{\partial K^0} - \frac{\partial \langle S^n(K^n(K^0)) \rangle_L}{\partial K^0} + ... \\
+[(K^n-K^*)-(K^m-K^*)] \partial \langle S^n(K^n \text{ or } m) \rangle_L + \frac{s}{\partial K^0} \text{ for } \langle K^n \text{ or } m \rangle.
\]

(3.18)

This becomes of practical use when \([\ ]\) becomes small because \(K^n-K^m\) is small compared to \((K_c-K^0)\) in this regime allowing a better estimate of \(K_c\) to be made if we have an approximate one already.

If we wish to simulate with the nearest neighbour Ising model and also wish to flow to \(K^*\) the fixed point of the RG transformation, then \(K_c\) must have the form \(K_c = (K_{nn,c}, 0, 0, ..., 0)\). With successive blockings starting from \(K_c\) (i.e. in the critical surface) then the relevant perturbations remain zero, and the irrelevant perturbations are decreased by factors \(b^i\) on each blocking, the system thus flowing to the fixed point and the transient correction terms tending to zero. For small deviations in \(K_{nn}\) so that we start close to but not at \(K_{nn,c}\) then the relevant perturbation is amplified by a factor of \(b^{i*} = b^{1/2} \sim 3\) for \(b = 2\) in the 3 d Ising model, on each application of blocking while the leading irrelevant correction is reduced by a factor \(b^{-\nu} \sim 1/2\) so that the accuracy in the \(K_{nn,c}\) estimate obtained from (3.18) increases potentially by a factor \(b\) at each blocking. Thus the best estimate for \(K_{nn,c}\) is obtained using equation (3.18) with \(n\) and \(m\) as large as possible and inverting the 1 x 1 matrix , in the \(K_{nn}\) subspace. Including other correlation functions allows estimates of points in the critical hypersurface with other coupling types to be obtained. This enables the entire critical hypersurface to be mapped out in principle. Thus equation (3.18) is very useful for finding improved starting points in the sense that they are closer to the fixed point so that irrelevant corrections are smaller. To exploit it all we have to do is to decide what kind of Hamiltonian we can accommodate then invert (3.18) with only terms included which correspond to the terms in the desired Hamiltonian. The irrelevant critical couplings are best obtained from the low RG levels while the relevant couplings are best tuned using the deepest RG levels.
Estimating the effective coupling constants

Wilson and Swendsen suggested small and large simulations of the same system as a method of measuring \textit{a posteriori} the effective, renormalised, coupling constants. The comparison of correlation functions on say 64 cubed blocked once and 32 cubed blocked no times gives an estimate of \(\{K^1\}\). This can be thought of in two ways: firstly the consequences of tuning \(K^0\) to \(K^0+(K^1-K^0)\) can be considered and correlation functions at \(K^1\) expressed as a Taylor series of correlation functions and derivatives at \(K^0\):

\[
<S^0(K^0+(K^1-K^0))>_s = <S^0(K^0)>_s + \alpha <S^0(K^0)>_s/\alpha K^0(K^1-K^0) + \ldots
\]  
(3.19)

The l.h.s. is the same as \(<S^1(K^1)>_L\) as the finite size effects are the same and the arguments are the same. Equally the consequences of tuning the RG transformation so that \(K^1+K^0+(K^1-K^0)\) can be explored to give:

\[
<S^1(K^1+K^0-K^1)>_L = <S^1(K^1)>_L+(K^0-K^1)d<S^1(K^1)>_L/dK^1
\]  
(3.20)

The l.h.s. is the same \(<S^0(K^0)>_s\). Either equations (3.19) and (3.20) can be inverted to give \(K^1\) knowing \(K^0\) to order \((K^1-K^0)^2\).

Averaging the results gives a better estimate true to order \((K^1-K^0)^2\), as does averaging the equations then inverting. The difference between averaging the results of (3.19) and (3.20) and the result given by averaging the equations before inverting gives a measure of the \((K^1-K^0)^3\) correction. To see the truth of these statements the quadratic and cubic terms in (3.19) and (3.20) must be kept in the analysis. Generalising (3.19) and (3.20) to any two lattice size comparisons with the larger system blocked \(n\) times and smaller system blocked \(m\) times so that the finite size effects are the same for \(<S^n>_L\) and \(<S^m>_s\) gives; in an implicit tensor notation for clarity,

\[
<S^n(K^n)>_L-<S^m(K^m)>_s = \alpha <S^n(K^n)>_L/\alpha K^n(K^n-K^m)
\]
\[-\frac{(K^n-K^m)}{2} \langle S^n(K^n) \rangle \leq \frac{\partial^2}{\partial K^m} \langle S^n(K^n) \rangle \]
\[+ \frac{(K^n-K^m)^3}{6 \partial^3} \langle S^n(K^n) \rangle \leq \frac{\partial^3}{\partial K^m} \langle S^n(K^n) \rangle + ... \]  
(3.21)

A similar equation is obtained by expanding the l.h.s. about \( K^m \): when the two equations are averaged the \( O(K^n-K^m)^n + 3 \) terms cancel, up to corrections of \( O(K^n-K^m)^3 \). This equation has been used to estimate the flow of coupling constants at each blocking level for \( K_{nn} \) (not necessarily \( K_{nn,0} \)). For example \{\( K^n \)\} can be calculated from 64 blocked once versus 32 blocked no times. Any residual finite size effects can be estimated from estimates of \{\( K^n \)\} from 32 blocked once versus 16 blocked no times. A table of available comparisons and the effective finite size effects is given below.

\[
\begin{array}{llll}
L = 64 & 64^0 & 64^1 & 64^2 & 64^3 & 64^4 & 64^5 \\
L = 32 & 64^0 & 64^1 & 64^2 & 64^3 & 64^4 & 64^5 \\
L = 16 & 64^0 & 64^1 & 64^2 & 64^3 & 64^4 & 64^5 \\
L = 8 & 64^0 & 64^1 & 64^2 & 64^3 & 64^4 & 64^5 \\
L = 4 & 64^0 & 64^1 & 64^2 & 64^3 & 64^4 & 64^5 \\
L = 2 & 64^0 & 64^1 & 64^2 & 64^3 & 64^4 & 64^5 \\
\end{array}
\]

**Figure (3.3): Available two lattice comparisons.**

The best estimates are obtained for \( (K^n-K^m) \) small and so are best for lattices differing by only 1 factor of \( b \) in size. Consistency checks can be made by comparing 643 blocked twice with 163 blocked no times etc., with the following possibilities:

\[
\begin{array}{llll}
64^2 & - (K^2) & \rightarrow 16^0 & 32^2 & - (K^2) & \rightarrow 8^0 \\
64^3 & - (K^3) & \rightarrow 16^1 & 32^3 & - (K^3) & \rightarrow 8^1 \\
64^4 & - (K^4) & \rightarrow 16^2 & 32^4 & - (K^4) & \rightarrow 8^2 \\
64^5 & - (K^5) & \rightarrow 16^3 \\
\end{array}
\]

**Figure (3.4): Available truncation estimates.**
The fixed point

A knowledge of the coupling constant flow with successive application of the chosen renormalisation transformation, e.g. majority rule, enables the position of the fixed point of this transformation to be estimated. Of course for any finite system, the maximum number of blockings is restricted to $L/2^n = 2$, say for scale factor $b = 2$. Thus the final coupling constants never quite reach $K'$. The resulting correction can be obtained via:

$$K'^n - K^{n+1} = T(K'^n - K^n)$$

which implies,

$$K'^n = (1 - T)^{-1}(K'^{n+1} - K^n)$$

(3.22)

where $T$ is the stability matrix as defined in equation (3.14). In practice the flow correction of order $O(K'^{n+1} - K^n)^3$ may be larger.

3.4. Results for the 3 d Ising model

As indicated earlier, the results for the coupling constant flow and the fixed point are obtained from an analysis of the data of Pawley et al (1984). The key equations are (3.19) and (3.20) for the coupling constant flow and (3.22) for the correction to obtain the fixed point. The various lattice comparisons of figure (3.3) are made.

We consider first the effective action estimates. Table (3.1) shows the output from $64^3$ versus $32^3$ comparisons. For the effective couplings after the first blocking starting from $K_{mn} = 0.22166$ (the best estimate for $K_{nn,0}$ is $0.221654(5)$ from Pawley et al (1984). Order $O(K'^{n+1} - K^n)^3$ corrections have been cancelled using the average of equations (3.19) and (3.20) before inverting.

Across the columns, we progress in blocking number, accumulating the calculated changes in coupling constants. The errors are obtained from a complete analyses of large (statistically independent) bins of data; this incorporates properly the potential benefit of the correlations of statistical errors between blocking levels. The rows represent the results of including an increasing operator basis in the matrix equations, specifically:
From the results we conclude the following. (1) There is substantial flow c.f. $K_{nn}$. (2) Most of the new couplings are stabilising rather satisfactorily as the number of operators included increases. (3) The $<200>$ operator is an important one both in its own right and in its effect upon the estimates for $K_{nn,c}$ and the fixed point and the coupling constant flow. This suggests that the naive hierarchy is not a sufficient guide to the inclusion order.

In order to obtain some estimate of the systematic uncertainty of neglecting $O(K^{n+1}-K^n)^3$, we show in table (3.2) the similar results obtained from inverting (3.19) and (3.20) separately to obtain independent estimates of the flow then averaging the results. There are significant differences at the blocking level and these accumulate for the final flow point estimate to as much as 4 or 5 standard deviations. Both methods are good to $O(K^{n+1}-K^n)^3$.

In table 3.3, we show the estimate for the fixed point $K^*$ using the “end correction” ((3.22)). We see that the “end correction” is tiny in comparison with the statistical uncertainty.

Finally, we show the coupling constant flow with all 7 operators included for $32^3$ versus $16^3$, to compare directly with Swendsen (1984), whose method will be indicated in the discussion on optimisation in the next chapter. Within the systematic uncertainty (neglect of $O(K^{n+1}-K^n)^3$) in our calculations the results agree and indeed we see that the average after inversion gives better agreement with Swendsen’s method for which the systematic errors should be smaller.

We conclude that the method in this chapter for coupling constant flow is viable and quantitatively accurate at least when the changes in renormalisation couplings are small; even with 20% changes in the coupling constants, the systematic discrepancy is around 2%.
\begin{table}[h]
\centering
\begin{tabular}{ccccccc}
\hline
\textbf{\(n=0\)} & \textbf{\(n=1\)} & \textbf{\(n=2\)} & \textbf{\(n=3\)} & \textbf{\(n=4\)} & \textbf{\(n=5\)} \\
\hline
0.221660 & (0) & 0.220803 & (17) & 0.221102 & (76) & 0.221514 & (272) & 0.222212 & (954) & 0.224582 & (3260) \\
0.221660 & (0) & 0.173220 & (51) & 0.168985 & (120) & 0.169995 & (254) & 0.170942 & (497) & 0.173067 & (1393) \\
0.000000 & (0) & 0.019389 & (24) & 0.021313 & (68) & 0.021054 & (194) & 0.020943 & (495) & 0.021060 & (1258) \\
0.221660 & (0) & 0.172182 & (52) & 0.167717 & (119) & 0.168653 & (245) & 0.169578 & (475) & 0.171696 & (1353) \\
0.000000 & (0) & 0.022707 & (34) & 0.026136 & (75) & 0.026512 & (144) & 0.026582 & (402) & 0.026851 & (917) \\
0.000000 & (0) & -0.003968 & (33) & -0.005918 & (87) & -0.006760 & (194) & -0.007003 & (429) & -0.006930 & (1000) \\
0.221660 & (0) & 0.169254 & (79) & 0.164632 & (168) & 0.164622 & (322) & 0.165291 & (981) & 0.168345 & (3241) \\
0.000000 & (0) & 0.022834 & (36) & 0.028329 & (79) & 0.025741 & (150) & 0.026820 & (405) & 0.026852 & (905) \\
0.000000 & (0) & -0.003990 & (33) & -0.005813 & (88) & -0.006606 & (194) & -0.006830 & (427) & -0.006786 & (957) \\
0.000000 & (0) & 0.001572 & (35) & 0.002952 & (71) & 0.003851 & (133) & 0.004067 & (560) & 0.003375 & (1779) \\
0.221660 & (0) & 0.170483 & (76) & 0.164632 & (168) & 0.165291 & (981) & 0.166136 & (3552) & \\
0.000000 & (0) & 0.022379 & (36) & 0.025624 & (79) & 0.025919 & (153) & 0.026006 & (416) & 0.025010 & (956) \\
0.000000 & (0) & -0.003772 & (33) & -0.005639 & (88) & -0.006415 & (194) & -0.006637 & (430) & -0.006601 & (990) \\
0.000000 & (0) & 0.000536 & (37) & 0.001333 & (75) & 0.001917 & (125) & 0.002168 & (339) & 0.001402 & (1011) \\
0.000000 & (0) & 0.001879 & (25) & 0.002930 & (52) & 0.003410 & (113) & 0.003377 & (414) & 0.003459 & (1055) \\
0.221660 & (0) & 0.170125 & (84) & 0.163912 & (187) & 0.163753 & (354) & 0.164373 & (961) & 0.167235 & (2996) \\
0.000000 & (0) & 0.021789 & (39) & 0.024612 & (84) & 0.025008 & (170) & 0.025132 & (538) & 0.025244 & (1326) \\
0.000000 & (0) & -0.003588 & (33) & -0.005395 & (88) & -0.006139 & (190) & -0.006375 & (414) & -0.006369 & (839) \\
0.000000 & (0) & 0.000132 & (39) & 0.000785 & (79) & 0.001309 & (132) & 0.001578 & (305) & 0.000866 & (839) \\
0.000000 & (0) & 0.001448 & (28) & 0.002355 & (56) & 0.002772 & (110) & 0.002764 & (362) & 0.002899 & (874) \\
0.000000 & (0) & 0.002467 & (46) & 0.003356 & (88) & 0.003709 & (205) & 0.003601 & (638) & 0.003326 & (1515) \\
0.221660 & (0) & 0.172696 & (92) & 0.167084 & (200) & 0.167130 & (384) & 0.167918 & (1049) & \\
0.000000 & (0) & 0.024515 & (49) & 0.028614 & (108) & 0.029152 & (184) & 0.029391 & (536) & \\
0.000000 & (0) & 0.001524 & (33) & 0.001592 & (75) & 0.001388 & (132) & 0.001221 & (351) & \\
0.000000 & (0) & 0.000132 & (45) & 0.000795 & (88) & 0.001318 & (148) & 0.001582 & (325) & \\
0.000000 & (0) & 0.001043 & (29) & 0.001791 & (59) & 0.002148 & (116) & 0.002130 & (371) & \\
0.000000 & (0) & 0.002066 & (48) & 0.002779 & (96) & 0.003063 & (214) & 0.002943 & (647) & \\
0.000000 & (0) & -0.012623 & (36) & -0.017091 & (94) & -0.018440 & (233) & -0.018868 & (501) & \\
\hline
\end{tabular}
\caption{Flow \(K^n\) via averaging equations then inverting. \(2 \times 10^6 \text{ m}^3/\text{s}\)}
\end{table}
Table (3.2): $K^n$ flow by inversion then averaging.

2.4x10^{6} \text{MCS/s}
Table (3.3): Fixed point, $K^*$, using the "end" correction.

<table>
<thead>
<tr>
<th>$n = 0$</th>
<th>$n=1$</th>
<th>$n=2$</th>
<th>$n=3$</th>
<th>$n=4$</th>
<th>$n=5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.221660 (0)</td>
<td>0.22203 (11)</td>
<td>0.220638 (20)</td>
<td>0.220887 (34)</td>
<td>0.221165 (83)</td>
<td>0.221154 (222)</td>
</tr>
<tr>
<td>0.221660 (0)</td>
<td>0.153641 (264)</td>
<td>0.169923 (374)</td>
<td>0.169931 (671)</td>
<td>0.170515 (1271)</td>
<td>0.171436 (2220)</td>
</tr>
<tr>
<td>0.221660 (0)</td>
<td>0.24774 (96)</td>
<td>0.021801 (137)</td>
<td>0.020852 (251)</td>
<td>0.020711 (479)</td>
<td>0.020335 (889)</td>
</tr>
<tr>
<td>0.221660 (0)</td>
<td>0.158902 (403)</td>
<td>0.167109 (543)</td>
<td>0.169600 (882)</td>
<td>0.169696 (1489)</td>
<td>0.172536 (2423)</td>
</tr>
<tr>
<td>0.221660 (0)</td>
<td>0.00231 (192)</td>
<td>0.005970 (252)</td>
<td>0.007552 (377)</td>
<td>0.007608 (739)</td>
<td>-0.010052 (1680)</td>
</tr>
</tbody>
</table>

**Table (3.3):** Fixed point, $K^*$, using the "end" correction.
Two lattice comparison, $L=32 \land L=16$, successively including more operators in $(3.19)$ and $(3.20)$.

<table>
<thead>
<tr>
<th>$n=0$</th>
<th>$n=1$</th>
<th>$n=2$</th>
<th>$n=3$</th>
<th>$n=4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.221660 (0)</td>
<td>0.220657 (12)</td>
<td>0.221110 (55)</td>
<td>0.221642 (211)</td>
<td>0.221885 (808)</td>
</tr>
<tr>
<td>0.221660 (0)</td>
<td>0.171418 (73)</td>
<td>0.167392 (179)</td>
<td>0.188632 (309)</td>
<td>0.169310 (667)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.020166 (32)</td>
<td>0.022096 (87)</td>
<td>0.021781 (193)</td>
<td>0.021574 (495)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.169748 (75)</td>
<td>0.165515 (182)</td>
<td>0.166677 (309)</td>
<td>0.167365 (669)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.024028 (47)</td>
<td>0.027474 (107)</td>
<td>0.027802 (219)</td>
<td>0.027663 (398)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>-0.004391 (33)</td>
<td>-0.006388 (76)</td>
<td>-0.007253 (245)</td>
<td>-0.007355 (544)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.166571 (87)</td>
<td>0.160373 (196)</td>
<td>0.159474 (349)</td>
<td>0.158747 (1055)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.024365 (48)</td>
<td>0.027897 (109)</td>
<td>0.028295 (220)</td>
<td>0.028207 (402)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>-0.004275 (33)</td>
<td>-0.006169 (77)</td>
<td>-0.006878 (251)</td>
<td>-0.006940 (557)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.002580 (40)</td>
<td>0.004441 (99)</td>
<td>0.006191 (211)</td>
<td>0.007250 (659)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.165281 (94)</td>
<td>0.158256 (217)</td>
<td>0.157150 (395)</td>
<td>0.156335 (1144)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.023860 (50)</td>
<td>0.027069 (113)</td>
<td>0.027274 (228)</td>
<td>0.027212 (405)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>-0.004117 (35)</td>
<td>-0.005964 (80)</td>
<td>-0.006705 (256)</td>
<td>-0.006783 (584)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001390 (38)</td>
<td>0.002381 (96)</td>
<td>0.003333 (190)</td>
<td>0.004215 (542)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001111 (39)</td>
<td>0.001905 (97)</td>
<td>0.002726 (195)</td>
<td>0.003573 (286)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001674 (37)</td>
<td>0.002580 (101)</td>
<td>0.003579 (225)</td>
<td>0.003774 (501)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.165908 (94)</td>
<td>0.159351 (220)</td>
<td>0.158617 (388)</td>
<td>0.157909 (1065)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.023432 (48)</td>
<td>0.026315 (108)</td>
<td>0.026277 (223)</td>
<td>0.026047 (420)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>-0.003988 (35)</td>
<td>-0.005728 (81)</td>
<td>-0.006374 (261)</td>
<td>-0.006431 (580)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001111 (39)</td>
<td>0.001905 (97)</td>
<td>0.002726 (195)</td>
<td>0.003573 (522)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001753 (29)</td>
<td>0.002381 (96)</td>
<td>0.003333 (190)</td>
<td>0.004215 (279)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001674 (37)</td>
<td>0.002852 (101)</td>
<td>0.003579 (225)</td>
<td>0.003774 (501)</td>
</tr>
<tr>
<td>0.221660 (0)</td>
<td>0.168526 (107)</td>
<td>0.162724 (249)</td>
<td>0.162435 (441)</td>
<td>0.162435 (467)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.026415 (60)</td>
<td>0.026315 (108)</td>
<td>0.026277 (223)</td>
<td>0.026047 (268)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001256 (38)</td>
<td>0.001299 (91)</td>
<td>0.000835 (251)</td>
<td>0.000835 (195)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.001076 (38)</td>
<td>0.001856 (93)</td>
<td>0.002862 (166)</td>
<td>0.002862 (166)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.000229 (34)</td>
<td>0.002165 (84)</td>
<td>0.002750 (116)</td>
<td>0.002750 (116)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>0.0001076 (39)</td>
<td>0.002016 (109)</td>
<td>0.002711 (234)</td>
<td>0.002711 (234)</td>
</tr>
<tr>
<td>0.000000 (0)</td>
<td>-0.013144 (56)</td>
<td>-0.017650 (118)</td>
<td>-0.01777 (219)</td>
<td>-0.01777 (219)</td>
</tr>
</tbody>
</table>

(a) Two lattice comparison, inverting $(3.19)$ and $(3.20)$, then averaging. $L=32 \land L=16, 4 \times 10^6$ MCS/s, $10$ MCS/avg.

(b) Swendsen's flow using Callen's representation (see p106). $4 \times 10^5$ MCS/s, $10$ MCS/avg.
Table (3.4): Swendsen’s $K^n$ versus Wilson’s two lattice comparison for $L = 32$. $K_{nn} = 0.22166$. Table (3.4)(a) shows the flow $K^n$, obtained using Wilson’s two lattice comparison method, while Table (3.4)(b) shows the flow Swendsen obtained using Callen’s representation. Comparison of the standard deviations for these different methods shows Swendsen’s method using Callen’s representation gives the same accuracy but with 10% of the run time.
4.1. Introduction

The MCRG method as described with extensions to allow coupling constant flow to be calculated has been very successfully applied to the calculation of critical exponents, renormalised couplings, the position of the fixed point and for mapping out the critical hypersurface (see for example Pawley et al. (1984)). The convergence of exponent estimates with blocking level is, however, often slow due to the presence of transient corrections to scaling, making extrapolation to an infinite number of blockings rather difficult. In this chapter we consider how the effects of corrections to scaling might be minimised in an MCRG simulation. Particularly we review a recent idea due to Swendsen (1984) which attempts to systematically remove the effect of slow transient corrections to scaling and hence improve the convergence of leading critical exponent estimates, by optimising the RSRG transformation in a so called optimised MCRG (OMCRG) simulation. An OMCRG for the 3 d Ising model is presented. The preliminary results indicate that as it stands our OMCRG simulation is not offering the enhanced convergence of exponents seen by Swendsen for a RSRG kernel weight function different only in the more weakly coupled operators. In order to analyse exactly what our optimised weight function is doing a new method suggested by Swendsen (1984) is invoked to follow the induced coupling constant flow. This is the state of the research completed. We intend in the near future to calculate the scaling fields with the truncation correction procedure of Shankar and Gupta (1985) included in the analysis and hence to calculate $d^{(n)}_{12} = \sum u^{n}_{i,j}$ the “distance” from the fixed point after n blockings for various RSRG weight factors.

What is optimisation?

Consider the space of all Ising Hamiltonians parameterised by an infinite set of couplings $K$. Provided we start in the critical hypersurface of the Ising Universality Class then we are guaranteed, after an infinite number of
blockings, to arrive at the Ising fixed point since by definition there are no other fixed points in this hypersurface by assumption. For a finite number of blockings we can only hope that the renormalised Hamiltonian, $H^n$, is very similar to the fixed point Hamiltonian, $H^\infty$. How similar is best measured by the scaling fields $u^n$ at the $n^{th}$ blocking level which are in general curvilinear co-ordinates. Excluding computational efficiency optimisation is taken to mean minimising the effect corrections to scaling have upon on quantities of interest.

In general the corrections to scaling enter estimates for quantities as shown in the equation below for a RSRG derivation of the susceptibility.

$$\chi^2(t,u_1,u_2,u^3...) = b^{n_1} + b^{n_2} + b^{n_3} + \ldots$$

$$\{1 + \sum_{i=1}^{n} b^{n_i} \partial(A(0,0..))/\partial(u_i b^i)/A(0,0..) + \ldots\}$$

where $b$ is the RSRG rescaling factor and $n$ the number of applications of the RSRG. The universal constants $A(0,0..)$ and its derivative can be obtained in terms of $G(K)$ as shown in van Leeuwen and Niemeijer (1976). In estimating leading exponents of the susceptibility by finite size scaling or series analysis or by MCRG what eventually prevents one from obtaining good estimates is lack of control over the miriad of irrelevant scaling fields in (4.1). Setting all the irrelevant fields to zero is how an MCRG performed at the fixed point would solve this. Fisher and Chen examined models with a free parameter which could be tuned to get them on to one of the so-called principal axes defined by $u_i=0$. The best we can do for as far as susceptibility is concerned is to minimize $\{ \}$. We are in general interested in many different quantities. In this case we do best to minimize the distance $d^2$ from the fixed point, which as suggested by Shankar (1985) is best measured by

$$d^{(n)^2} = \sum_i u_i^{(n)^2}$$

which correctly takes account of possible curvature of the critical hypersurface in the space of effective coupling constants.
**Improved Action**

The idea of simulating with an improved action as first suggested by Ma (1976), is to perform the simulation closer to the fixed point and hence in n RSRG levels get closer than before to the fixed point. Simulation at the fixed point will for a general RSRG transformation require the complete set of couplings which are embeddable in the lattice. The number of couplings in this set increases dramatically with lattice size. For a small number of couplings m, Swendsen (1980) has suggested the way to proceed is to make the deviations from the fixed point in the direction of the right eigenvectors corresponding to the m largest eigenvalues vanish. In this way the effect of transient irrelevant perturbations should be reduced, $T|K^\alpha$ give a better estimate to $T|K^\alpha$, the linear approximation rendered increasingly valid and measured quantities exhibit the critical behaviour expected with smaller corrections to scaling.

How many couplings can practically be included in the updating algorithm and how many are needed to secure a place in the hypersurface closer to the fixed point than $\{K_{nn,c}0,0,0,\ldots\}$? The answer to the second question is provided in part by the results of chapter 3 on coupling constant flow for several even and odd couplings. The question of practicality is postponed to chapter 5 where a comparison of update times for, 4 coupling and 16 coupling actions using Metropolis and demon algorithms, is made.

Suppose we want to perform a MCRG simulation with an improved action and say a majority rule RSRG weight function. A knowledge of the fixed point and the right eigenvectors in a basis of spin operators measured in a previous MCRG with majority rule allows the equations,

$$\sum_{\alpha} \phi_{i\alpha}(K_{\alpha} - K^\alpha) = u_i, \quad (4.3)$$

to be used together with the criterion adopted for "closeness" to calculate the couplings and their values to include in the Improved Action. As a zeroth approximation we can simply place the equations so that scaling fields corresponding to the largest exponent are uppermost in the hierarchy of inclusion. We can then chose to set the first m couplings to their fixed point values (best estimates from table (3.4) with all measured correlation functions included) and live with the remaining n-m couplings set to zero. This gives...
for m=4 the following 4 term improved action:

\[ K_1 = 0.16398(239) \ <100> \text{ spin operator} \]
\[ K_2 = 0.02612(79) \ <110> \text{ spin operator} \]
\[ K_3 = -0.00440(271) \ <111> \text{ spin operator} \]
\[ K_4 = -0.00391(852) \ <200> \text{ spin operator}. \]

The danger with this zeroth approximation is that if these 4 couplings do not saturate the leading scaling field then the n-m couplings set to zero constitute a perturbation, \( \sum \phi_{iQ}(0-K^Q_{\alpha}) \), out of the critical hypersurface (there are of course further possible corrections due to fields we have not measured which we are here formally assuming to be zero).

A better procedure is to set \( u_1 \) to zero and minimise \( \sum u_i^{(n)2} \) subject to \( K_5, K_n=0 \). This could be implemented using a least squares fitting routine. Instead we use the estimates in table (3.3) chapter 3 obtained by inverting equation (3.) in the subspace of the first four operators. The best estimate for \( K_1 \) comes from the deepest blocking level, while the 1st blocking level gives the best estimates for \( K_2, K_3 \) and \( K_4 \) corresponding to the approximate truth, verified by the flow for majority rule, that \( K_1 \) dominates the contributions to \( u_1 \) and where as \( K_n, n>1 \) contribute mostly to the irrelevant scaling fields \( u_n, n>1 \). The 4 couplings obtained are

\[ K_1 = 0.221693(62) \]
\[ K_2 = 0.000177(8) \]
\[ K_3 = -0.000158(8) \]
\[ K_4 = 0.000336(11) \]

The implementation of an improved action requires the following modifications to the configuration generating routine described in chapter 2. The detailed balance condition requires that none of the spins connected through the Hamiltonian are simultaneously updated and so several planes need to be merged together to obtain a full planes worth of spins to update. The look up table of course grows considerably. For the 4 coupling improved action

\[ H(\sigma) = K_1 S_{<100>} + K_2 S_{<110>} + K_3 S_{<111>} + K_4 S_{<200>} \] (4.4)

the Metropolis algorithm
\[ P(\sigma_i'=-\sigma_i,\sigma_i) = \exp(+\Delta H) \quad \Delta H < 0 \]
\[ 1 \quad \Delta H \geq 0 \]  
(4.5)

requires the following single spin flip energy change to be calculated

\[ \Delta H(\sigma_i) = -2\sigma_i[K_1\sum \sigma_j + K_2\sum \sigma_j + K_3\sum \sigma_j + K_4\sum \sigma_j] \]  
(4.6)

for which the terms have 7, 13, 9, and 7 possible neighbour counts respectively. Consequently the transition matrix can be constructed as a look table with 7.13.9.7 entries which are addressed using the counts for each term as a label.

The feasability of this algorithm is examined in chapter 5 where implementation costs are considered.

4.2. Optimising the RSRG in MCRG

Swendsen has suggested that the freedom of choice of the weight function of the RSRG transformation might be exploited to make a desired Hamiltonian, say the 3 d Ising model, a fixed point of that transformation. In principle the complete set of operators embeddable in the lattice, just as with the improved action simulation, are needed in general to make the the model of our choice a fixed point. In this way he hoped to perform a simulation as close to the fixed point as an improved action simulation but absorb the extra couplings needed into a set of “optimised” parameters in the RSRG transformation thus removing practically all the extra computing costs from the updating algorithm into the RSRG algorithm which is only called on the configurations chosen for measurement.

**Possible forms for a tunable RSRG transformation**

In general an RSRG transformation can be defined as:

\[ \exp(K^{n+1}S^{n+1}G^{n+1}) = \]
where \( \{ \sigma^{n+1} \} \) is produced by the action of the projection operator \( P(\sigma^{n+1}, \sigma^n) \) on \( \{ \sigma^n \} \). The spin independent constants in this definition can be removed by using equation (1.21) from chapter 1 to divide the left hand side by \( Z^{n+1} \) and the right hand side by \( Z^n \) and then identifying \( \exp(K^nS^n+G^n)/\sum \exp(K^nS^n+G^n) \) (in which we see the constants \( G^n \) cancel) as the probability \( p(\sigma^n) \) of obtaining the blockspin configuration \( \sigma^n \). Thus we rephrase the RSRG transformation as:

\[
p(\sigma^{n+1}) = \sum_{\{\sigma'^n\}} P(\sigma^{n+1}, \sigma^n)p(\sigma^n)
\]

Here as in chapter 1 blocking is chosen to involve reducing the number of degrees of freedom by \( b^d \) to produce a configuration of blockspins on a lattice isomorphic to the unblocked spin lattice but of \( b \) times the lattice spacing. A correlation length scaling argument suggests that only spins within \( \xi \) of a subject spin (one about to blocked) affect that subject spin and hence the operators determining the blockspins should not need to extend beyond \( \xi \) spatially. This is the heuristic argument that an RSRG transformation should be local and need only extend to the correlation length of the system. The correlation length of our simulation must be \( \leq L \) and so each subject spin is determined by the local pattern of spins less than or equal to \( \xi \) or \( L \) whichever is the smaller. This is a key assumption and will be questioned later. The locality assumption also suggests that a subject blockspin depends most strongly on the pattern of spins nearby and less progressively on the more distant pattern. How quickly this series can be truncated is questionable and though spins distant from the subject blockspin interact weakly there are an increasingly large number of such spins (a bit like Olber's paradox). Which effect wins is the question.

We use the same parameterisation for the weight function as Swendsen:

\[
P(\sigma^{n+1}, \sigma^n) = \prod_j P_j(\sigma_j^{n+1}, \sigma^n)
\]

which restricts the resultant RSRG transformation to be of a local nature. The site dependent weight functions are chosen to be
\[
\begin{align*}
\tilde{R}_{\alpha,j}(\sigma^n) &= \exp(\sigma^{n+1}_i \sum \rho_{\alpha} \hat{R}_{\alpha,j}(\sigma^n)/2 \cosh(\sum \rho_B \hat{R}_{B,j}(\sigma^n))) \\
\text{(4.10)}
\end{align*}
\]

where \( \hat{R}_{\alpha,j}(\sigma^n) \) is defined by the choice of \( \sigma^{n+1}_i \hat{R}_{\alpha,j}(\sigma^n) \) as an even symmetric combination of spins centred around \( \sigma^{n+1}_i \) and including it. In particular Swendsen choses the \( \hat{R}_{\alpha,j} \)'s so that they depend on \( \sigma^n \) only through the combination \( \hat{R}_0 \), the majority rule operator of block cell \( j \). Where \( \hat{R}_0 \) is undetermined because of a tie it is not allowed to contribute to the RSRG weight function. In this way \( \hat{R}_{\alpha,j}(\sigma^n) \) can be regarded as a function defined on the majority rule determined blocked lattice of blocked lattice. This choice simplifies the quantities needed to calculate derivatives with respect to \( \rho \) formally and also makes the RSRG a small perturbation about majority rule.

If the method is to work it should turn out that the first few most important operators \( \hat{R}_{\alpha,j} \) such as \( \hat{R}_{nn,j}, \hat{R}_{nnn,j} \) dominate the sum in the exponential single spin RSRG weight function and that the \( \rho_{\alpha} \) tend to zero as \( \alpha \) becomes larger corresponding to less local \( \hat{R}_{\alpha,j} \). In general an infinite set of all possible operators embeddable on the blocked lattice is required. The tuning would then indicate what values are required for \( \rho_{nn} \), etc... It is important to define a complete set of operators. An overcomplete set leads to equivalence of certain operators and associated eigenvalues and eigen-operators. An under complete set means truncation effects may be serious. There is a lot of room for experimenting with what finite set of operators are best to include. For an even Hamiltonian the choice of even RSRG transformation ensures that the \( T \) matrix separates out into even and odd block diagonal form thus preserving the even ness of the original Hamiltonian.

The constraints:

\[
1 \geq P(\sigma^{n+1},\sigma^n) = 0
\]

and

\[
\sum_{\{\sigma^{n+1}\}} P(\sigma^{n+1},\sigma^n) = 1
\]

ensure
\[ Z^{n+1} = Z^n \]  
(4.13)

which can be checked explicitly for the choice \((4.10)\) The dependence of correlation functions on the RSRG transformation via the \(\rho\)'s can be investigated in the vicinity of \(\{\rho^*\}\) where the Hamiltonian required becomes the fixed point. The resulting formal derivatives allow the/an optimal set of \(\{\rho^*\}\) of RSRG parameters to be found systematically from measurements made during a simulation.

\[ \langle S^{n+1}(K^{n+1},\rho) \rangle = \sum_{\xi^{n+1}} S^{n+1}(\sigma^{n+1}) \]
\[ \exp(K^{n+1}S^{n+1}) \sum_{\xi^{n+1}} \exp(K^{n+1}S^{n+1}) \]  
(4.14)

where \(K^{n+1}\) will depend on the \(K^n\) through \(\rho\) and ultimately on \(K^0\). Using \((4.7)\) to feed in the RSRG transformation we obtain

\[ \langle S^{n+1}(K^{n+1},\rho,K^0) \rangle = \sum_{\xi^{n+1}} S^{n+1}(\sigma^{n+1}) \]
\[ \exp(K^0S^n) \sum_{\xi^{n+1}} K^0S^n \]  
(4.15)

and then Taylor expanding about \(\rho^*\) gives:

\[ \langle S^{n+1}(\rho+(\rho^* - \rho)) \rangle = \langle S^{n+1}(\rho) \rangle \]
\[ + (\rho^* - \rho) \partial \langle S^{n+1}(\rho) \rangle / \partial \rho^* \]  
(4.16)

where for the specific parameterisation the derivative can be formally evaluated to give

\[ \partial \langle S^{n+1}_\alpha \rangle / \partial \rho_\beta = \sum_{\xi^{n+1}} \langle S^{n+1}_\alpha \rangle \]
\[ \{ \sum_{\xi}(\sigma^{n+1} - \tanh(\rho_i R^{n+1}))R_B^{n+1} \} \]  
(4.17)

there being no disconnected piece because we have via \((4.8)\) defined the RSRG
as acting on \( p(\sigma) \) rather than \( \exp(H(\sigma)) \). Equation (4.17) allows us to calculate the optimised couplings. Deeper blocking levels also give an estimate for \( p^* \) to be found which is very sensitive and provides a consistency check on the values found. Callen's representation \([\text{Callen (1963)}]\) affords a means of monitoring the couplings for different RSRG transformations by integrating out one spin in the definition for a canonical average to obtain, with the minimum of labour, an expectation value with an explicit \( K \) dependence:

\[
<S_{\alpha}^{n+1}(K;\rho,K)> = \frac{1}{m_{\alpha}}
\]
\[
\sum_j <S_{\alpha,i}(\sigma^{n+1}) \tanh(\kappa S_j^{n+1}(\sigma^{n+1})>
\]

(4.18)

where the \( m_{\alpha} \) is the spin multiplicity and is included to avoid over counting. The \( K \) have replaced \( K' \) and indicate the guess currently being made for the couplings. The guess can be systematically improved by formally calculating the derivative of \( \partial <S_{\alpha}> / \partial K_B \) as is done below. Callen's representation is also affected by the RSRG transformation in operation, the extent to which it is sensitive to each parameter is given by:

\[
<S(\rho^* - \rho; K)> =
\]
\[
<S(\rho; K)> + \partial <S(\rho; K)> / \partial \rho +...
\]

(4.19)

If \( K \) needs to be adjusted to give \( K^*=(K_{nn,c},0,0,...) \), the required fixed point then an extra correction term should be included so that (4.16) becomes:

\[
<S_{\alpha}(\rho^* - \rho; K + (K_{nn,c} - K))>
\]
\[
<S_{\alpha}(\rho; K)> + \partial <S_{\alpha}(\rho; K)> / \partial \rho (K_{nn,c} - K)
\]

(4.20)

The new \( \rho \)'s can be found systematically provided \((\rho - \rho^*)\) is not too large. Combining (4.16), (4.19) and (4.20) gives:
\[
\langle S^{n+1}(K^{n+1}; \rho) \rangle - \langle S^{n+1}(K^{n+1}; \rho; K) \rangle = \\
[\partial <S(K^{n+1}; \rho; K)>/\partial \rho - \partial <S^{n+1}(K^{n+1}; \rho)>/\partial \rho \rangle (\rho^* - \rho) \\
+ \partial <S(K^{n+1}; \rho; K)>/\partial K_j (K_{nn,c} - K) + .. \tag{4.21}
\]

The flow is monitored using the formal derivative of Callen's representation in

\[
\langle S^{n+1}(K^{n+1}) \rangle - \langle S^{n+1}(K^{n+1}, K) \rangle = \\
\partial <S^{n+1}(K^{n+1}; K)>/\partial K + .. \tag{4.22}
\]

4.3. The OMCRG performed at Edinburgh

The blocking rule parameterisation of equation (4.5) has been implemented on the DAP for the 3 d Ising model (as usual) on a simple cubic lattice with periodic boundary conditions for lattice size L=8 and 16 while code exists for L=32, 64, and 128. The code generates configurations using fast DAPFORTRAN Metropolis algorithms for the small systems and the code of Reddaway et al for L=64 and 128. As a preliminary test we have simulated on L=8 with \( K_{nn} = 0.22166 \) and a so-called "majority rule plus tiebreaker" blocking procedure which is as follows. A configuration chosen for blocking is divided up into coarse-grained cells (constituencies) of \( b^d \) spins (voters) and a blockspin (MP) chosen (elected) to be "up" (labour) or "down" (conservative) if the majority of spins are "up" or "down" respectively. In the event of a tie in cell \( j \) the parameterisation (4.5) is invoked to determine the blockspin. In Swendsen's paper the tiebreaking on cell \( j \) is determined by the local pattern of majority rule determined blockspins. Where the local coarse-grained cells are also in need of a tiebreak they are disqualified from tiebreaking. The values taken by the parameters \( p \) are at the discretion of the programmer who decides upon the RSRG rule (constitution). In Swendsen's implementation the \( \hat{R}_i(\sigma^n) \) thus depend only on the majority rule determined blockspins denoted by \( \sigma_{k}^{n+1} = \hat{R}_{j; k} (\sigma^n); \in k = \text{sign}(\sum \sigma_{i}^{n}) \). The \( \hat{R}_{Q,j}(\sigma^{n+1}) \) have been chosen so as to sample the coarse grained cell pattern symmetrically.
Clearly many other choices of tiebreak are conceivable. Obvious choices are to soften majority rule and have $\rho_0$ large but finite. This would require doing a majority rule to generate a set of probable blockspins then $p_0 \hat{R}_j(0^n)$ on this probable blockspin configuration would completely determine the actual blockspin pattern. Equally the operators might be defined on the site spin configuration to be blocked rather than the majority rule determined probable (or partial) blockspin configuration. This would seem a fairer suggestion for conducting an election where your vote counts not only in your constituency but also in the symmetrically distributed constituencies in the vicinity though probably with a reduced weighting.

With a particular blocking strategy chosen the set of $\hat{R}_j$ to include is a matter of physical intuition. We tried a set based on the following hierarchy of 2 spin 4 spin 6 spin etc... and within a set of $n$ spin operators ordering according to locality. In principle the order of importance should be

$$\text{order} = (K_{c,nn} - K^2) \sum_{\alpha} \langle p_{\alpha} - p_{\alpha}^* \rangle$$

and hence reflect the component in the direction of the vector connecting $K^*_{c}$ of the universality class with the desired simulation point.

The set of tiebreaking operators chosen is given in order of expected "importance", together with the set used by Swendsen. The labelling convention is to call the block spin cell $j$ the origin and then to use cartesian co-ordinates to indicate the position of the other spins in $\hat{R}_{B,j}$. This gives one of the spin combinations contributing to the topology $\hat{R}_{B,j}$. The others are obtained by summing over the symmetric set of such topologies connected to site $j$. It is important that spin combinations used are symmetric about the site they effect. Another trick is to permute the origin of the blockspin cell through all $b^d=8$ possibilities preferably numbering the corners of this cube so that successive origins are not connected through the Hamiltonian.
\[ \hat{R}_{j,\alpha} \]

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>terms</th>
<th>number of terms</th>
<th>normalised to</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(000,100)</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>2</td>
<td>(000,110)</td>
<td>6</td>
<td>12</td>
</tr>
<tr>
<td>3</td>
<td>(000,111)</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>(000,200)</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>(100,210)</td>
<td>12</td>
<td>24</td>
</tr>
<tr>
<td>6</td>
<td>(000,211)</td>
<td>12</td>
<td>24</td>
</tr>
<tr>
<td>7</td>
<td>(000,220)</td>
<td>6</td>
<td>12</td>
</tr>
<tr>
<td>8</td>
<td>(000,221)</td>
<td>12</td>
<td>24</td>
</tr>
<tr>
<td>9</td>
<td>(000,222)</td>
<td>4</td>
<td>8</td>
</tr>
</tbody>
</table>

4 spin operators

<table>
<thead>
<tr>
<th></th>
<th>terms</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>(000,100,110,010)</td>
<td>12</td>
</tr>
<tr>
<td>11</td>
<td>(000,110,111,001)</td>
<td>24</td>
</tr>
<tr>
<td>12</td>
<td>(000,100,010,091)</td>
<td>8</td>
</tr>
<tr>
<td>13</td>
<td>(000,100,110,010)</td>
<td>4</td>
</tr>
<tr>
<td>14</td>
<td>(000,110,101,011)</td>
<td>8</td>
</tr>
</tbody>
</table>

6 spin operators

<table>
<thead>
<tr>
<th></th>
<th>terms</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>(000,100,200,210,110,010)</td>
<td>12</td>
</tr>
</tbody>
</table>

8 spin operator

<table>
<thead>
<tr>
<th></th>
<th>terms</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>(000,100,110,010,001,101,111,011)</td>
<td></td>
</tr>
</tbody>
</table>

Table (44): The tiebreaking operator set.

In each case the smallest symmetric set of terms is kept.

The correlation function measurements need only sample each topology once for each direction \( x,y,z \) and over all lattice sites. The set of measured correlation functions is the same as in table (4.1).

The mapping of the systems onto the DAP copied exactly those described in chapter 2 care being exercised to respect any interleaving. Details of the extensive code will be published at a later date.

From the basic measurements \( \hat{S}_{j,\alpha}^{n+1}(\sigma^n) \) and \( \hat{R}_{j,\alpha}(\sigma^n) \) for the various RSRG levels \( n \) the following ensemble averages were constructed:
4.4. Preliminary results

Firstly the results of the L=8 simulation at $K_{nn,c}=0.22166$ are presented. A well equilibrated configuration was used and 16 bins of $2^{16}2$ measurements with 20 MCS/S between successive measurements made for $p=(0.0,0.0...)$ i.e., majority rule. This gave a check of the code by comparison of the correlation functions with Pawley et al and an initial estimate of the p's required to make $K_{nn,c}$ a stationary point. (I drop the term fixed point since we are not sure that $K_{nn}$ can be made a fixed point in the RSRG sense). These are in agreement with Swendsen though on a smaller lattice. The coupling constant flow $\tilde{\alpha}$ la Swendsen is obtained and agrees with the results of two lattice comparison method. These p's and K's are presented in table (4.2).

A second iteration was performed using as input the p's of table (4.2). With a further $2^{16}13312$ measurements the improved estimates were obtained as shown in table (4.3). We note the p's seem to converge to a well defined vector The coupling constant flow indicates that indeed even using the first iteration estimates for $p$ that the flow has been stemmed and $K_{nn,c}$ is a stationary point within statistical error. A third iteration of the same number of measurements gives table (4.4), confirming that the method homes in on a unique set of optimal parameters.

Summarising the results for L=8 we conclude:

(1) A unique set of p's emerges which are stable to inclusion of an
increasing basis of operators.

(2) Callen's representation is an excellent method for following coupling constant flow particularly when $\mathcal{K}$ is close to the actual coupling constants. The inclusion of 16 operators does indicate that the truncation to the 7 measured operators of Pawley et al in chapter 3 is rather brutal.

(3) Successive iterations quickly converge on a set $\rho^*$ which agree with Swendsen and which Callen's representation confirms makes $K_{nn}$ a stationary point.

The eigenvalues for the first three iterations of $L=8$ are shown in Table (4.5). Across the table the $\rho$ are improved starting on the left hand side with majority rule and ending on the right with the best estimate of $\rho^*$. Down the table the blocking level increases from $n=1$ ($L/b^2=4$) to $n=2$ ($L/b^2=2$). The convergence and the values are not markedly different for the three iterations, though there is a hint that the $T$ matrix is slightly more diagonal since the $1^*1$ value is not so different from $2^*2$ etc... values. The inclusion of more operators makes a significant difference as Pawley et al suggested.

A similar set of tables are listed for $L=16$ except no majority rule is presented there. The trends are the same as the $L=8$ though the small finite size effects are at work and render the $\rho$ in better agreement with Swendsen. The eigenvalues do not exhibit the enhanced convergence seen by Swendsen.

Conclusions

Recently there has been an exchange of comments between Fisher and Randeria (1986) and Swendsen (1986) concerning the OMCRG letter of Swendsen (1984). In order to make explicit the issues raised I use the RSRG derivation of the free energy as given in van Leeuwen and Niemeijer (1976). Thus I endeavour to examine the totality of explanations for Swendsen's enhanced convergence and our zero enhancement.

For a RSRG calculation to give the critical exponents there must be a non-trivial fixed point $K^*$ about which $K'(K)$ must be analytic. To calculate $f(K)$, the integration constants generated by RSRG for each length scale removed, $g(K)$, must also be regular and in a large domain of $K$ space. In terms of scaling fields $u$ and $g(u)$ (whose functional form differs from $g(K)$ of course and is given in principle by substituting $K(u)$ in $g(K)$; similarly $f(u)$ and $f(K)$) the assumptions become that $u=0$ corresponds to a non-trivial fixed point, that
u(K) is regular in the K domain of interest and that g(u) be regular. With these assumptions one obtains:

\[ f(u_1, u_2, u_3 \ldots) = \sum_{n_1, n_2, \ldots} \alpha_n \]

\[ g_{n_1,n_2,n_3,u_1^n u_2^{n_2}/(1-b^-d \lambda_1^n \lambda_2^{n_2})} + |u_1|^{-d/y_1} \sum_{n=0}^{\infty} \alpha_n^\pm |u_1|^{2\pi \ln/\log \lambda_1} \]  

(4.24)

where the \( \alpha_n^\pm \) are given by,

\[ \alpha_n^\pm = 1/\log \lambda_1 \int_0^\infty dt/t^{1+d/y_1} \]

\[ \left. g_{\text{rem}}(u_2|u_1|^{-\gamma_2/y_1 t^{\gamma_2/y_1} t_2^{\gamma_3/y_3}}) t^{-2\pi \ln/\log \lambda_1} \right|_{\gamma_2} \]  

(4.25)

and

\[ g_{\text{rem}}(x,y,z \ldots) = \sum_{n_1,n_2 \ldots} g_{n_1,n_2 \ldots u_1^n u_2^{n_2}} \]  

(4.26)

The first term is the regular contribution the free energy the second the singular part.

Consider a physical quantity, say the zero field susceptibility, near the fixed point, \( \lambda^* \), of the majority rule RSRG transformation, denoted by \( R \), on a critical Ising system. The susceptibility in this region is given by

\[ \chi^{(2)}(u_1,u_2 \ldots) = |u_1|^{-d+y_2/y_1} \]

\[ \sum_{n=0}^{\infty} \partial \alpha^\pm_n (u_2/u_1|^{\gamma_2/y_1 \ldots}) / \partial (u_2/u_1)^{y_2/y_1}) \]  

(4.27)

where the scaling fields are given by the matrix of derivatives via

\[ u_i = \sum_{\alpha} \phi_i \alpha (K_\alpha - K^* \alpha) + \ldots \]  

(4.28)
where $\phi_{i, \alpha}$ are the components of the left eigen-vector corresponding to the eigenvalue $\lambda_i$. The axis along which corrections to scaling vanish is given by,

$$u_i = 0 \ i=3,4,... \ i.e.. \ correction \ to \ scaling \ fields.$$

defining the so-called principal axis in $K$ space. Now consider our new RSRG transformation $R^+$ with a fixed point $K^+$ which may $a \ priori$ differ from $K^*$ (since the fixed point is non-universal). The scaling fields for this $R^+$ are

$$u_i^+ = \sum_{\alpha} \phi_i^{+\alpha}(K^\alpha - K^* \alpha) \tag{4.29}$$

and the susceptibility is given by

$$\chi^{(2)}(u_1^+, u_2^+, \ldots) = |u_1|^{-(d+\gamma_2^+)/(\gamma_1)}$$

$$\exists A^{\pm} = \partial(u_2^+/|u_1|^{\gamma_2^+/(\gamma_1^+)}) (0,0,0,...)$$

$$\{1+e A^{\pm} = \partial(u_3^+/|u_1|^{\gamma_3^+/(\gamma_1^+)}) (0,0,0,...)\}$$

Now the susceptibility $\chi^{(2)}(u) = \chi^{(2)}(K)$ is a physical quantity and so $R$ and $R^+$ must give the same $\chi(K)$ for all $K$ especially in the domain of interest. So we obtain, simplifying the constants

$$|u_1|^\gamma A$$

$$\{1 + Bu_3 |u_1|^{-\gamma_3/(\gamma_1^+)} = |u_1|^\gamma A^+$$

$$\{1 + B^+ u_3 |u_1|^{-\gamma_3^+/(\gamma_1^+)} \}$$

an equation relating the $g_{n_1 n_2 \ldots}^\alpha$ of $R^+$; $\phi_i, i=1,\ldots$, and $\lambda_i, i=1,\ldots$ of RSRG transformation $R$ to the corresponding $'+'$ quantities for $R^+$.

For a non-singular RSRG transformations $R$ and $R^+$ the implications are: $K^+ = K^*$: $u_i = 0 \rightarrow u_i^+ = 0$ for all $i$; $\gamma_i = \gamma_i^+$ for all $i$. In words the fixed points for two
non-singular RSRG transformations, the exponents governing the scaling towards these fixed points and the various axes defined by \( u_i = 0 \) and the values taken by the universal functions \( A, B, A^+, \text{and } B^+ \) at the fixed point are the same. For \( K \) not equal to the fixed point or corresponding to a point on any one of the principle axes the eigenvectors the universal functions \( A, B, A^+ \) and \( B^+ \) and the values taken by \( u(K) \) and \( u^K(K) \) differ.

The suggestion then is that if the Swendsen ORG is non-singular then the fixed point is not actually moved but the scaling fields warped into highly non-linear functions of \( K \) so that the linear approximations involved in calculating the coupling constant flow give the impression of a stationary nearest neighbour Hamiltonian. If this is the case the true distance from the fixed point for a given blocking level for the two Rs as measured by the scaling field flow, \( u^0 \), if compared with the coupling constant distance \( K^0 - K^* \) will indicate the non-linearity.

As far as accelerated convergence with blocking level is concerned the key quantity is \( u^{(n)} \) for the various RSRG transformations tried. If we can organise for to be \( u^{(n)} = a(K^{n} - K^*) + b(\ )^2 + c(\ )^3 \) then small flow from \( (K_{nn}, c, 0, 0) \) towards \( K^* \) will yield a large flow in terms of the scaling field. To implement this procedure extensions beyond the linear regime are required.

The other possibilities are that the RSRG transformation is singular such that \( u_1 = u_2 = u_3 \). But for this to be true for all \( K \) either \( K^* = K^* \) or \( y_i = y_i^* \) is a function of \( K \) via \( u^* \). It is possible, because the \( Q(K) \) terms cancel in the definition of the RG transformation, that these can be singular without causing any damage to the stability matrix.

There are cases where an overcomplete basis of \( K \) renders some points in this space physically the same. In such cases an RSRG transformation generating a flow between the two equivalent \( K^* \) would give a bogus redundant [ Wegner (1976); Shankar and Gupta (1985)] eigenvalue which could be mistaken for a physical eigenvalue rather than the artefact of the RSRG scheme implementation. There is no reason to believe \( K^* \) and \( (K_{nn}, c, 0, 0) \) are physically equivalent points. An optimisation scheme might be envisaged which notes the redundant equivalents of the fixed point and where the system being simulated is closer to the redundant image point a redundant transformation performed to ensure flow to that point.
Tables of results

$\rho_{\alpha}^O$: The optimised RSRG weight function parameters

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>n=0</th>
<th>n=1</th>
<th>n=2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\infty$</td>
<td>$\infty$</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0.0000</td>
<td>0</td>
<td>-0.1570</td>
</tr>
<tr>
<td>2</td>
<td>0.0000</td>
<td>0</td>
<td>0.0794</td>
</tr>
<tr>
<td>3</td>
<td>0.0000</td>
<td>0</td>
<td>0.0343</td>
</tr>
<tr>
<td>4</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0259</td>
</tr>
<tr>
<td>5</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0073</td>
</tr>
<tr>
<td>6</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0023</td>
</tr>
<tr>
<td>7</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0044</td>
</tr>
<tr>
<td>8</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0014</td>
</tr>
<tr>
<td>9</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0011</td>
</tr>
<tr>
<td>10</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0106</td>
</tr>
<tr>
<td>11</td>
<td>0.0000</td>
<td>0</td>
<td>-0.0019</td>
</tr>
<tr>
<td>12</td>
<td>0.0000</td>
<td>0</td>
<td>0.0364</td>
</tr>
<tr>
<td>13</td>
<td>0.0000</td>
<td>0</td>
<td>0.0005</td>
</tr>
<tr>
<td>14</td>
<td>0.0000</td>
<td>0</td>
<td>0.0011</td>
</tr>
</tbody>
</table>

$K_{\alpha}$: effective coupling constant generated by $\rho_{\alpha}^O$

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>n=0</th>
<th>n=1</th>
<th>n=2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.22170</td>
<td>17</td>
<td>0.16259</td>
</tr>
<tr>
<td>2</td>
<td>0.00001</td>
<td>11</td>
<td>0.02877</td>
</tr>
<tr>
<td>3</td>
<td>-0.00001</td>
<td>9</td>
<td>0.00625</td>
</tr>
<tr>
<td>4</td>
<td>-0.00013</td>
<td>11</td>
<td>-0.00612</td>
</tr>
<tr>
<td>5</td>
<td>0.00001</td>
<td>7</td>
<td>-0.00221</td>
</tr>
<tr>
<td>6</td>
<td>0.00000</td>
<td>5</td>
<td>-0.00089</td>
</tr>
<tr>
<td>7</td>
<td>0.00004</td>
<td>7</td>
<td>-0.00038</td>
</tr>
<tr>
<td>8</td>
<td>0.00002</td>
<td>5</td>
<td>-0.00019</td>
</tr>
<tr>
<td>9</td>
<td>-0.00017</td>
<td>8</td>
<td>-0.00014</td>
</tr>
<tr>
<td>10</td>
<td>-0.00003</td>
<td>9</td>
<td>0.00166</td>
</tr>
<tr>
<td>11</td>
<td>-0.00004</td>
<td>6</td>
<td>0.00113</td>
</tr>
<tr>
<td>12</td>
<td>-0.00008</td>
<td>5</td>
<td>0.00272</td>
</tr>
<tr>
<td>13</td>
<td>0.00006</td>
<td>5</td>
<td>0.00080</td>
</tr>
<tr>
<td>14</td>
<td>0.00014</td>
<td>5</td>
<td>0.00095</td>
</tr>
</tbody>
</table>

Table (4.2): First iteration starting from majority rule plus a random tiebreaker on $L=8$ with $K_{mn}=0.22166$, 2,621,440 MCS/S in total and 20 MCS/S between measurements.
\( \rho^{(n)}_{\alpha} \): The optimised RSRG weight function parameters

\[
\begin{array}{cccccc}
\alpha & n=0 & n=1 & n=2 & & \\
0 & \infty & 0 & \infty & 0 & \infty \\
1 & 0.15709 & 0 & 0.15824 & 16 & 0.15858 \\
2 & -0.07944 & 0 & -0.07874 & 4 & -0.08245 \\
3 & -0.03433 & 0 & -0.03702 & 20 & -0.03753 \\
4 & 0.02591 & 0 & 0.02861 & 7 & 0.00000 \\
5 & 0.00731 & 0 & 0.00715 & 3 & 0.00000 \\
6 & 0.00239 & 0 & 0.00169 & 4 & 0.00000 \\
7 & 0.00446 & 0 & 0.00465 & 7 & 0.00000 \\
8 & 0.00145 & 0 & 0.00162 & 2 & 0.00000 \\
9 & 0.00110 & 0 & 0.00130 & 4 & 0.00000 \\
10 & 0.01064 & 0 & 0.00900 & 9 & 0.00834 \\
11 & 0.00199 & 0 & 0.00175 & 5 & 0.00199 \\
12 & -0.03640 & 0 & -0.03352 & 11 & -0.03353 \\
13 & -0.00057 & 0 & -0.00069 & 3 & 0.00000 \\
14 & -0.00116 & 0 & -0.00130 & 9 & -0.00082 \\
\end{array}
\]

\( \kappa^{(n)}_{\alpha} \): Effective coupling constants generated by \( \rho^{(n+1)} \) from the 1\(^{st} \) iteration.

\[
\begin{array}{cccccc}
\alpha & n=0 & n=1 & n=2 & & \\
1 & 0.22157 & 8 & 0.22118 & 30 & 0.2182 \\
2 & 0.00004 & 6 & -0.00356 & 12 & 0.00050 \\
3 & -0.00007 & 5 & 0.00260 & 22 & 0.0046 \\
4 & 0.00005 & 6 & -0.00410 & 14 & 0.00000 \\
5 & -0.00000 & 3 & 0.00124 & 7 & 0.00000 \\
6 & -0.00001 & 2 & 0.00050 & 7 & 0.00000 \\
7 & 0.00003 & 3 & 0.00048 & 11 & 0.00000 \\
8 & -0.00000 & 2 & -0.00012 & 7 & 0.00000 \\
9 & 0.00002 & 4 & 0.00011 & 6 & 0.00000 \\
10 & 0.00006 & 5 & 0.00030 & 20 & 0.0043 \\
11 & -0.00001 & 3 & 0.00030 & 11 & -0.00002 \\
12 & -0.00005 & 4 & -0.00187 & 7 & -0.0016 \\
13 & -0.00001 & 3 & 0.00033 & 8 & 0.00000 \\
14 & 0.00001 & 7 & 0.00042 & 22 & 0.00000 \\
\end{array}
\]

Table (4.3): The 2\(^{nd} \) iteration on L=8 using \( \rho^{(n+1)} \) from the 1\(^{st} \) iteration with 8,519,680 MCS/S and 20MCS/S between measurements.
\( \rho_{\alpha}^{(n)} \): The RSRG weight function parameters with \( \rho^{(n+1)} \) from the 2nd iteration used as the starting point for this third iteration.

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( n=0 )</th>
<th>( n=1 )</th>
<th>( n=2 )</th>
<th>( n=3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( 0.15728 )</td>
<td>( 0.15807 )</td>
<td>( 0.15810 )</td>
<td>24</td>
</tr>
<tr>
<td>1</td>
<td>( -0.07907 )</td>
<td>( -0.07847 )</td>
<td>( -0.08183 )</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>( -0.03587 )</td>
<td>( -0.03838 )</td>
<td>( -0.03879 )</td>
<td>14</td>
</tr>
<tr>
<td>3</td>
<td>( 0.02781 )</td>
<td>( 0.03015 )</td>
<td>( 0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>( 0.00714 )</td>
<td>( 0.00704 )</td>
<td>( 0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>( 0.00191 )</td>
<td>( 0.00132 )</td>
<td>( 0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>( 0.00471 )</td>
<td>( 0.00485 )</td>
<td>( 0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>( 0.00157 )</td>
<td>( 0.00171 )</td>
<td>( 0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>( 0.00133 )</td>
<td>( 0.00141 )</td>
<td>( 0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>( 0.00987 )</td>
<td>( 0.00854 )</td>
<td>( 0.00761 )</td>
<td>13</td>
</tr>
<tr>
<td>10</td>
<td>( 0.00191 )</td>
<td>( 0.00180 )</td>
<td>( 0.00191 )</td>
<td>5</td>
</tr>
<tr>
<td>11</td>
<td>( -0.03472 )</td>
<td>( -0.03249 )</td>
<td>( -0.03167 )</td>
<td>15</td>
</tr>
<tr>
<td>12</td>
<td>( -0.00001 )</td>
<td>( -0.00011 )</td>
<td>( -0.00000 )</td>
<td>0</td>
</tr>
<tr>
<td>13</td>
<td>( -0.00003 )</td>
<td>( -0.00004 )</td>
<td>( -0.00000 )</td>
<td>0</td>
</tr>
</tbody>
</table>

\( K_{\alpha}^{(n)} \): The effective coupling constants generated by the \( \rho^{(n)} \) of the third iteration.

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( n=0 )</th>
<th>( n=1 )</th>
<th>( n=2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( 0.22161 )</td>
<td>( 0.22171 )</td>
<td>( 0.21955 )</td>
</tr>
<tr>
<td>1</td>
<td>( 0.00001 )</td>
<td>( 0.00319 )</td>
<td>( 0.00501 )</td>
</tr>
<tr>
<td>2</td>
<td>( 0.00000 )</td>
<td>( 0.00257 )</td>
<td>( 0.00428 )</td>
</tr>
<tr>
<td>3</td>
<td>( -0.00004 )</td>
<td>( -0.00359 )</td>
<td>( 0.00000 )</td>
</tr>
<tr>
<td>4</td>
<td>( 0.00000 )</td>
<td>( 0.00107 )</td>
<td>( 0.00000 )</td>
</tr>
<tr>
<td>5</td>
<td>( 0.00000 )</td>
<td>( 0.00046 )</td>
<td>( 0.00000 )</td>
</tr>
<tr>
<td>6</td>
<td>( 0.00001 )</td>
<td>( 0.00029 )</td>
<td>( 0.00000 )</td>
</tr>
<tr>
<td>7</td>
<td>( -0.00002 )</td>
<td>( -0.00263 )</td>
<td>( 0.00000 )</td>
</tr>
<tr>
<td>8</td>
<td>( -0.00002 )</td>
<td>( 0.00029 )</td>
<td>( 0.00000 )</td>
</tr>
<tr>
<td>9</td>
<td>( 0.00005 )</td>
<td>( 0.00145 )</td>
<td>( 0.00176 )</td>
</tr>
<tr>
<td>10</td>
<td>( 0.00004 )</td>
<td>( 0.00036 )</td>
<td>( 0.00000 )</td>
</tr>
</tbody>
</table>

Table (4.6): 3rd iteration on L=8 with starting point \( \rho^{(n+1)} \) from 2nd iteration, \( K_{\alpha}^{(n)}=0.22166 \), 10,485,760 MCS/S and 20MCS/S between measurements.
Renormalisation group exponents for three iterations (RSRG weight functions) $y_i(p)$

<table>
<thead>
<tr>
<th>n=1 first blocking level</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.411</td>
<td>0.004</td>
<td>1.433</td>
<td>0.001</td>
<td>1.431</td>
</tr>
<tr>
<td>-0.472</td>
<td>0.056</td>
<td>-0.480</td>
<td>0.037</td>
<td>-0.441</td>
</tr>
<tr>
<td>-1.534</td>
<td>0.058</td>
<td>-1.565</td>
<td>0.029</td>
<td>-1.638</td>
</tr>
<tr>
<td>-1.534</td>
<td>0.062</td>
<td>-2.898</td>
<td>0.144</td>
<td>-1.703</td>
</tr>
<tr>
<td>-3.145</td>
<td>0.196</td>
<td>-3.619</td>
<td>0.132</td>
<td>-3.365</td>
</tr>
<tr>
<td>-3.145</td>
<td>0.109</td>
<td>-3.619</td>
<td>0.092</td>
<td>-3.365</td>
</tr>
<tr>
<td>-3.499</td>
<td>0.227</td>
<td>-4.132</td>
<td>0.110</td>
<td>-3.641</td>
</tr>
<tr>
<td>-3.499</td>
<td>0.162</td>
<td>-4.275</td>
<td>0.227</td>
<td>-3.641</td>
</tr>
<tr>
<td>-4.644</td>
<td>0.160</td>
<td>-5.350</td>
<td>0.368</td>
<td>-4.804</td>
</tr>
<tr>
<td>-4.800</td>
<td>0.272</td>
<td>-5.787</td>
<td>0.488</td>
<td>-4.804</td>
</tr>
<tr>
<td>-4.800</td>
<td>0.742</td>
<td>-7.137</td>
<td>0.440</td>
<td>-5.470</td>
</tr>
<tr>
<td>-10.287</td>
<td>0.739</td>
<td>-10.287</td>
<td>0.320</td>
<td>-10.287</td>
</tr>
<tr>
<td>-10.287</td>
<td>0.722</td>
<td>-10.287</td>
<td>0.511</td>
<td>-10.287</td>
</tr>
<tr>
<td>-10.287</td>
<td>0.001</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

n=2 second blocking level (2 cubed blocked configuration)

<table>
<thead>
<tr>
<th></th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.645</td>
<td>0.002</td>
<td>1.675</td>
<td>0.001</td>
<td>1.676</td>
</tr>
<tr>
<td>-1.362</td>
<td>0.021</td>
<td>-1.314</td>
<td>0.014</td>
<td>-1.405</td>
</tr>
<tr>
<td>-1.775</td>
<td>0.049</td>
<td>-1.715</td>
<td>0.025</td>
<td>-1.749</td>
</tr>
<tr>
<td>-4.010</td>
<td>0.114</td>
<td>-3.527</td>
<td>0.095</td>
<td>-3.395</td>
</tr>
<tr>
<td>-4.010</td>
<td>0.125</td>
<td>-3.988</td>
<td>0.074</td>
<td>-3.957</td>
</tr>
<tr>
<td>-4.489</td>
<td>0.193</td>
<td>-5.051</td>
<td>0.152</td>
<td>-4.873</td>
</tr>
<tr>
<td>-5.088</td>
<td>0.396</td>
<td>-5.295</td>
<td>0.226</td>
<td></td>
</tr>
</tbody>
</table>

odd eigenvalues

n=1 first blocking level

<table>
<thead>
<tr>
<th></th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.458</td>
<td>0.001</td>
<td>2.443</td>
<td>0.031</td>
<td>2.505</td>
</tr>
<tr>
<td>0.108</td>
<td>0.007</td>
<td>0.126</td>
<td>0.096</td>
<td>0.230</td>
</tr>
</tbody>
</table>

-118a-
Table (4.5): Eigenvalues resulting from 1st, 2nd and 3rd iterations of the $\varphi$ used in the RSRG blocking rule for $L=8$ and $k_m = 0.22166$. Standard deviations for 1st, 2nd and 3rd iterations are given in columns 2, 4 and 6 respectively.

<table>
<thead>
<tr>
<th></th>
<th>1st Iteration</th>
<th>2nd Iteration</th>
<th>3rd Iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta = 2$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.471</td>
<td>0.001</td>
<td>2.502</td>
<td>0.0004</td>
</tr>
<tr>
<td>0.206</td>
<td>0.004</td>
<td>0.239</td>
<td>0.0038</td>
</tr>
</tbody>
</table>

2nd blocking level
\( \rho_{\alpha}^{(\rho)} \): The optimised RSRG weight function parameters

\[
\begin{array}{cccccc}
\alpha & n=0 & n=1 & n=2 & n=3 \\
\hline
0 & \infty & \infty & \infty & \infty & \infty \\
1 & 0.15079 & 0 & 0.15724 & 4 & 0.16004 & 15 & 0.15886 & \infty & \infty \\
2 & -0.07944 & 0 & -0.07904 & 4 & -0.08057 & 10 & -0.08213 & \infty & \infty \\
3 & -0.03433 & 0 & -0.03585 & 3 & -0.03935 & 28 & -0.03763 & \infty & \infty \\
4 & 0.02591 & 0 & 0.02784 & 4 & 0.03004 & 15 & 0.00000 & \infty & \infty \\
5 & 0.00731 & 0 & 0.00714 & 1 & 0.00764 & 4 & 0.00000 & \infty & \infty \\
6 & 0.00239 & 0 & 0.00193 & 2 & 0.00164 & 6 & 0.00000 & \infty & \infty \\
7 & 0.00446 & 0 & 0.00475 & 2 & 0.00505 & 9 & 0.00000 & \infty & \infty \\
8 & 0.00145 & 0 & 0.00155 & 1 & 0.00185 & 4 & 0.00000 & \infty & \infty \\
9 & 0.00110 & 0 & 0.00135 & 2 & 0.00145 & 4 & 0.00000 & \infty & \infty \\
10 & 0.01064 & 0 & 0.00965 & 2 & 0.00935 & 11 & 0.00815 & \infty & \infty \\
11 & 0.00199 & 0 & 0.00193 & 1 & 0.00175 & 5 & 0.00205 & \infty & \infty \\
12 & -0.03640 & 0 & -0.03475 & 4 & -0.03495 & 18 & -0.03395 & \infty & \infty \\
13 & -0.00057 & 0 & -0.00065 & 1 & -0.00065 & 3 & 0.00000 & \infty & \infty \\
\end{array}
\]

\( K_{\alpha}^{(\rho)} \): The effective coupling constants generated by \( \rho_{\alpha}^{(n=0)} \)
of 1st iteration of L=16.

\[
\begin{array}{cccccc}
\alpha & n=0 & n=1 & n=2 & n=3 \\
\hline
1 & 0.2216 & 6 & 0.22246 & 11 & 0.21658 & 41 & 0.2176 & 18 \\
2 & 0.0001 & 3 & -0.00311 & 8 & -0.00074 & 26 & 0.0002 & 6 \\
3 & 0.0004 & 3 & 0.00347 & 10 & 0.00364 & 33 & 0.0049 & 3 \\
4 & 0.0002 & 4 & -0.00471 & 9 & -0.00569 & 21 & 0.0000 & 0 \\
5 & -0.0005 & 1 & 0.00128 & 4 & 0.00096 & 9 & 0.0000 & 0 \\
6 & 0.0000 & 2 & 0.00041 & 6 & 0.00029 & 13 & 0.0000 & 0 \\
7 & 0.0000 & 2 & 0.00002 & 6 & 0.00062 & 15 & 0.0000 & 0 \\
8 & 0.0000 & 1 & 0.00032 & 6 & -0.00027 & 11 & 0.0000 & 0 \\
9 & -0.0000 & 2 & -0.00022 & 8 & 0.00021 & 8 & 0.0000 & 0 \\
10 & 0.0000 & 4 & 0.00239 & 9 & 0.00378 & 26 & 0.0052 & 7 \\
11 & -0.0000 & 2 & 0.00006 & 3 & 0.00114 & 12 & -0.0001 & 2 \\
12 & 0.0000 & 2 & -0.00190 & 6 & -0.00661 & 14 & -0.0009 & 2 \\
13 & -0.0000 & 2 & 0.00025 & 6 & 0.00054 & 11 & -0.0000 & 0 \\
\end{array}
\]

Table (4.6): 1st iteration of L=16 using \( \rho_{\alpha}^{(n=1)} \)
of 1st iteration of L=8.

-119-
The optimised RSRG weight function parameters.

\[ \rho^{(n)}_{\alpha} \]: The effective coupling constants generated by \( \rho^{(n)}_{\alpha} \) from the 1st L=16 iteration.

\[ K^{(n)}_{\alpha} \]: The effective coupling constants generated by \( K^{(n)}_{\alpha} \) from the 1st L=16 iteration.

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( n=0 )</th>
<th>( n=1 )</th>
<th>( n=2 )</th>
<th>( n=3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( \infty )</td>
<td>( \infty )</td>
<td>( \infty )</td>
<td>( \infty )</td>
</tr>
<tr>
<td>1</td>
<td>0.15728</td>
<td>0</td>
<td>0.1573</td>
<td>7</td>
</tr>
<tr>
<td>2</td>
<td>-0.07907</td>
<td>0</td>
<td>-0.0787</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>-0.03587</td>
<td>0</td>
<td>-0.0370</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>0.02781</td>
<td>0</td>
<td>0.0294</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>0.00714</td>
<td>0</td>
<td>0.0070</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>0.00191</td>
<td>0</td>
<td>0.0014</td>
<td>2</td>
</tr>
<tr>
<td>7</td>
<td>0.00471</td>
<td>0</td>
<td>0.0048</td>
<td>3</td>
</tr>
<tr>
<td>8</td>
<td>0.00157</td>
<td>0</td>
<td>0.0016</td>
<td>1</td>
</tr>
<tr>
<td>9</td>
<td>0.00133</td>
<td>0</td>
<td>0.0015</td>
<td>4</td>
</tr>
<tr>
<td>10</td>
<td>0.00987</td>
<td>0</td>
<td>0.0091</td>
<td>2</td>
</tr>
<tr>
<td>11</td>
<td>0.00191</td>
<td>0</td>
<td>0.0018</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>-0.03472</td>
<td>0</td>
<td>-0.0331</td>
<td>4</td>
</tr>
<tr>
<td>13</td>
<td>-0.00063</td>
<td>0</td>
<td>-0.0007</td>
<td>2</td>
</tr>
</tbody>
</table>

Table: The 2nd iteration of L=16 using \( \rho^{(n=1)}_{\alpha} \) of L=16 1st iteration. 2,621,440 MCS/S, 20 MCS/measurement.
The table below shows the eigenvalues resulting from 1st and 2nd iterations of $\rho$ used in the RSRG blocking rule for $L=16$ and $kn = 0.22166$. The 2nd and 4th columns list the errors in the values given in the 1st and 3rd columns respectively.
Explicit comparison with Swendsen's OMCRG

In table (4.9) below we compare the optimized parameters obtained by Swendsen for \(2.16 \times 10^6\) MCS/spin on \(L=16\) and \(K_{nn}=0.22166\) with our \(p\)s resulting from the 2nd iteration of \(L=16\) for which \(2.62144 \times 10^6\) MCS/spin were performed.

<table>
<thead>
<tr>
<th>Swendsen</th>
<th>Wall</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1592(6)</td>
<td>0.1573(7) (100)</td>
</tr>
<tr>
<td>-0.0762(3)</td>
<td>-0.0787(3) (110)</td>
</tr>
<tr>
<td>-0.0473(3)</td>
<td>-0.0370(4) (111)</td>
</tr>
<tr>
<td>0.0396(5)</td>
<td>0.0294(6) (200)</td>
</tr>
<tr>
<td>0.0025(3)</td>
<td>0.0070(2) (210)</td>
</tr>
<tr>
<td>-0.0044(3)</td>
<td>0.0014(2) (211)</td>
</tr>
<tr>
<td>0.0010(2)</td>
<td>0.0048(3) (220)</td>
</tr>
<tr>
<td>-0.0019(2)</td>
<td>0.0016(1) (221)</td>
</tr>
<tr>
<td>-0.0007(4)</td>
<td>0.0015(4) (222)</td>
</tr>
<tr>
<td>0.0040(4)</td>
<td>0.0091(2) (100,110,010)</td>
</tr>
<tr>
<td>0.0021(3)</td>
<td>0.0018(1) (100,010,001)</td>
</tr>
<tr>
<td>-0.0201(4)</td>
<td>-0.0331(4) (111,110,001)</td>
</tr>
</tbody>
</table>

Table (4.9): Comparison of optimized parameters with those of Swendsen.

The agreement is quite good for the (100) and the (110) operators. The (111) and (200) operators have the same relative importance in both our and Swendsen's results though there is a significant discrepancy. The remaining operators have in both cases smaller optimized parameters as hoped though there does not seem to be much agreement between our \(p\) values and Swendsen's for these operators. We have included 1 extra operator in our \(L=16\) RSRG kernel and 2 extra operators in our \(L=8\) RSRG kernel. The discrepancies mentioned suggest that the inclusion of 1 or 2 "unimportant" operators can have a significant effect upon all but the (100) and the (110) operators. Another possibility is that there are many minima in \(p\) space corresponding to several distinct optimized parameter sets solving equation (4.21) and that Swendsen is one minimum while we are in another. Both these suggestions constitute a serious problem for the successful application of the method.

The leading eigenvalues corresponding to simulation with the \(p\)s of table (4.9) are now given together with the majority rule values obtained by Pawley.

$\nu_{11}$

<table>
<thead>
<tr>
<th>Swendsen</th>
<th>Wall</th>
<th>Pawley</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.08 $10^6$</td>
<td>2.62144 $10^6$</td>
<td>16 $10^6$ MCS/spin</td>
</tr>
</tbody>
</table>

$n=1$ eigenvalues from the first blocking level

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.506(2)</td>
<td>1.4007(18)</td>
<td>1.3655(3)</td>
</tr>
<tr>
<td>1.553(1)</td>
<td>1.4419(13)</td>
<td>1.4371(2)</td>
</tr>
<tr>
<td>1.558(1)</td>
<td>1.4414(14)</td>
<td>1.4376(3)</td>
</tr>
<tr>
<td>1.556(2)</td>
<td>1.4402(14)</td>
<td>1.4368(3)</td>
</tr>
<tr>
<td>1.556(2)</td>
<td>1.4350(15)</td>
<td>1.4330(4)</td>
</tr>
<tr>
<td>1.556(2)</td>
<td>1.4291(18)</td>
<td>1.4303(4)</td>
</tr>
<tr>
<td>1.555(3)</td>
<td>1.4195(23)</td>
<td></td>
</tr>
<tr>
<td>1.556(3)</td>
<td>1.4179(23)</td>
<td></td>
</tr>
<tr>
<td>1.558(3)</td>
<td>1.4168(24)</td>
<td></td>
</tr>
<tr>
<td>1.558(3)</td>
<td>1.4151(24)</td>
<td></td>
</tr>
<tr>
<td>1.558(2)</td>
<td>1.4145(22)</td>
<td></td>
</tr>
<tr>
<td>1.558(2)</td>
<td>1.4139(19)</td>
<td></td>
</tr>
<tr>
<td>1.558(2)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$n=2$

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.519(9)</td>
<td>1.5233(21)</td>
<td>1.5137(4)</td>
</tr>
<tr>
<td>1.588(8)</td>
<td>1.5744(23)</td>
<td>1.5656(6)</td>
</tr>
<tr>
<td>1.593(8)</td>
<td>1.5753(35)</td>
<td>1.5662(6)</td>
</tr>
<tr>
<td>1.590(8)</td>
<td>1.5638(24)</td>
<td>1.5556(6)</td>
</tr>
<tr>
<td>1.586(7)</td>
<td>1.5504(29)</td>
<td>1.5420(8)</td>
</tr>
<tr>
<td>1.585(9)</td>
<td>1.5365(29)</td>
<td>1.5399(8)</td>
</tr>
<tr>
<td>1.584(7)</td>
<td>1.5393(31)</td>
<td>1.5338(8)</td>
</tr>
<tr>
<td>1.584(9)</td>
<td>1.5323(29)</td>
<td></td>
</tr>
<tr>
<td>1.585(9)</td>
<td>1.5301(32)</td>
<td></td>
</tr>
<tr>
<td>1.586(9)</td>
<td>1.5296(33)</td>
<td></td>
</tr>
<tr>
<td>1.587(9)</td>
<td>1.5282(31)</td>
<td></td>
</tr>
<tr>
<td>1.585(9)</td>
<td>1.5284(31)</td>
<td></td>
</tr>
<tr>
<td>1.585(9)</td>
<td>1.5201(33)</td>
<td></td>
</tr>
</tbody>
</table>

$n=3$

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.7346(35)</td>
<td>1.6585(7)</td>
<td></td>
</tr>
<tr>
<td>1.7733(31)</td>
<td>1.7460(3)</td>
<td></td>
</tr>
<tr>
<td>1.7759(32)</td>
<td>1.7545(5)</td>
<td></td>
</tr>
<tr>
<td>1.7560(28)</td>
<td>1.7249(7)</td>
<td></td>
</tr>
<tr>
<td>1.7474(19)</td>
<td>1.7079(7)</td>
<td></td>
</tr>
<tr>
<td>1.7301(29)</td>
<td>1.7051(8)</td>
<td></td>
</tr>
</tbody>
</table>

Table (4.10): Comparison of leading even exponent, $\nu_1$. 
We do not see the improved convergence that Swendsen does. Neither is our data as stable as his as the operator basis used in equation (3.14) and (3.15) is increased. In fact our results converge only marginally better than the majority rule case despite the fact that blocked correlation functions do take the $K_{nn,c}$ values (checked by comparison with $K_{nn,c}$ simulations on lattices of appropriate size) indicating that $K_{nn,c}$ is a stationary point. We do not understand this discrepancy. Clearly somehow the matrix of derivatives is not the same for Swendsen and us, though the correlation functions $<S_{\alpha}^n>$ appear to be the same. It must be that operators of the form $<S_{\alpha}^nS_{\beta}^m>$ are different in our simulation to those of Swendsen. Higher statistics are needed to see this. The large difference in convergence and exponent values between Swendsen and ourselves suggests that the eigenvalues are very sensitive to the slight differences in optimized parameters. We did not expect this. The first thing to do to investigate the discrepancy must be to simulate with precisely Swendsen's operator set and with his set of optimized parameters to ensure we have faithfully implemented his procedure.

The leading odd eigenvalues are now tabulated in a similar way to table (4.10)
<table>
<thead>
<tr>
<th></th>
<th>Swendsen</th>
<th>Wall</th>
<th>Pawley</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_h$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>n=1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4461(2)</td>
<td>2.45963(4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4423(2)</td>
<td>2.45832(4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4418(2)</td>
<td>2.45789(7)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4417(2)</td>
<td>2.45831(7)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.45831(7)</td>
</tr>
<tr>
<td>2.502(?)</td>
<td></td>
<td></td>
<td>2.45831(7)</td>
</tr>
<tr>
<td>n=2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4752(4)</td>
<td>2.47721(12)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4579(5)</td>
<td>2.46291(14)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4562(6)</td>
<td>2.46188(13)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.4559(5)</td>
<td>2.46117(13)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.46116(13)</td>
</tr>
<tr>
<td>2.500(?)</td>
<td></td>
<td></td>
<td>2.46117(13)</td>
</tr>
<tr>
<td>n=3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.5481(12)</td>
<td>2.52542(39)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.5171(11)</td>
<td>2.48437(52)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.48236(54)</td>
</tr>
</tbody>
</table>

Table (4.11): Comparison of leading odd exponent, $\gamma_h$.

Our values for $\gamma_h$ are very similar to those by Pawley et al. Though the odd correlation functions differed from those of Pawley et al and were consistent with renormalised couplings $K^n = K_{n,c}^n, 0, 0...$. Swendsen's estimates for $\gamma_h$ are very sensitive to the optimized parameters, $\rho$, and are at odds with the estimate of Pawley et al.

In summary, we have not found the OMCRG method as successful as we had hoped. Whether the discrepancies with Swendsen's work can be reconciled will only emerge with further investigation.
CHAPTER 5

FAST ISING CODE

5.1. Introduction

The search for methods of obtaining good numerical estimates of thermodynamic averages in critical systems in a minimum of computer machine clock cycles is the motivation for this chapter. Extracting the most important information from the $2^N$ points in phase space can be done in many ways. The Demon algorithm affords a means of sampling phase space in a way which can interpolate between the microcanonical and canonical ensembles. On the one hand shrinking the demons to zero yields a MC method of simulating the microcanonical ensemble which on the ICL DAP has been optimised to achieve 1.75 Ghz (spin update attempts per second) for the 2d Ising model. On the other hand running a simulation with several types of demons, one for each of 4 couplings, allows a very fast simulation of the truncated 3d Ising improved action mentioned in chapter 4. The expected speed of the final code for 4 bit plane sack size demons (defined below) is 122 Mhz and for zero sack size demons (the microcanonical improved action) is 199 Mhz. As a spin off the fast algorithms provide objective ways of benchmarking computers for bit manipulation problems.

Creutz's Demons

A system of spins, say, is in thermal contact with one (or more) demon(s) [Creutz (1983)] the combined system being thermally isolated. The demon algorithm allows a walk through the combined phase space of lattice and demon configurations, \{\sigma,d\}, to be made in such a way as to preserve the total energy:

$$E_t = E(\sigma) + E_d(d)$$

(5.1)

The updating algorithm is as follows. A demon visits a lattice site and accepts the new trial state spin provided it can accommodate the change in lattice energy by suitably adjusting the demon energy in its sack. The sack must be
constrained to have a lower bound conveniently arranged to be zero to prevent the demon from running away with all the energy. An upper bound conveniently allows for faster computer code using integers or logicals. The demon is the mediator of energy transfer, as in Maxwell's demons, and can be instructed to sweep through the lattice sequentially or randomly. Table (5.1) summarises the demon algorithm.

initialise lattice+demon so that $E_s + E_d = E_t$

allow the demon to visit each site of the lattice sequentially or randomly

consider changing the chosen spin $\sigma_j$
to the single spin trial state $\sigma_j'$
calculate the energy, $E_d' = E_d + E - E'$
the new demon's sack will have if it agrees to accommodate the energy change
accept the trial state
iff $0 < E_d' = < n_{max}$ and adjust the sack contents to $E_d'$
so that the total energy of the system is conserved

move to the next spin and repeat.

Increasing the number of demons to a platoon or brigade allows for parallel updating to be performed with the precaution of detailed balance to ensure that the probability $\{\sigma,d\}<..>\{\sigma',d'\}$ are the same. In practice this means that spins connected through the Hamiltonian should not be simultaneously updated.

Variations on this method include allowing the demon to visit a heat bath in between updates and thereby have its energy reset to $E_d$ with probability $\exp(-\beta E_d)$ with $\beta$ the Boltzmann factor, which recovers the Metropolis algorithm. Equally, a randomly hopping demon locally reduces to the Metropolis algorithm because the contents of the demon sack are Boltzmann distributed by other sites before returning to update the same site. If the number of demons is very small then they act essentially as thermometers sampling the lattice energy fluctuations. The lattice energy in this limit is almost constant and the algorithm, using a parallel updating procedure, generates the microcanonical ensemble of lattice energy $E_s$, the demon playing the same role that conjugate momenta do in the microcanonical time
evolution of Hamilton's equations of motion. On the other hand the limit where
the number of demons greatly exceeds the number of lattice sites, or more
precisely $E_d >> E$, then the demon acts as a heat bath with which the lattice
exchanges energy. And so the heat bath algorithm is recovered. Extension of
the single sacked demon to a multi-sacked with say $m$ sacks with contents
denoted by $a_1 \ldots a_m$ allows a Hamiltonian of the form, $H(\sigma) = \sum \beta_i A_i(\sigma)$, to be
simulated with constraints imposed on each $A_i(\sigma)$ via the restrictions on
$a_1 \ldots a_m$. In the thermometer limit, $A_{i,d} << A$ for all $i$, allows a hunt through
$\{\sigma,d\}$ phase space with the following constraints, $A_{i}(\sigma)+a_{i}(\sigma)=A_{i,T}$ for all $i$. This allows effective couplings to be
found by $m$ single parameter hunts rather than a costly single $m$ parameter
hunt. Bhanot (1985) has illustrated the application of this method to tracking
RG flow in the 2d Pure Ising model on a square lattice with periodic boundary
conditions and a majority rule plus random number tiebreaker as the blocking
transformation.

The following references make explicit the connection between the demon
ensemble and the micro-canonical ensembles and provide examples of the
variety of physics accessible to demons. The ergodicity of the demon
Extension to multi-sacked demons is used in Bhanot (1985) to track MCRG
flow. The possibility of using demons to investigate heat flow is made real in
Creutz (1984b).

5.2. Very fast algorithms for generating Ising spin configurations

The problems of critical slowing down [Hohenberg and Halperin (1977)],
increased relaxation times, and increased spatial correlation lengths associated
with systems simulated at criticality demand very fast updating algorithms and
the use of powerful computers especially where large systems need to be
simulated. In particular a lot of effort has been spent developing fast Ising
model algorithms recently on various computers. As well as enabling high
precision numerical experiments these algorithms have also emerged as a
means of bench marking computer performance.

In this section we describe fastest algorithms developed at Edinburgh, which
bench mark the ICL DAP for: the Metropolis algorithm [Reddaway et al (1985)];
the 1 sacked and 4 sacked demon algorithms [Toral and Wool (1986)]; and the
zero sack demon or microcanonical ensemble [Toral and Wool (1986)]. The
algorithms are compared with the best developed on other machines and suggestions for further improvements and their theoretical timings presented.

**Fast Metropolis Algorithm for the Ising Model**

A complete description is provided by the originators, Reddaway et al (1985); here the basic features giving the speed up are briefly outlined. The algorithm consists of three parts:

- **stage (1)** random number generation;
- **stage (2)** nearest neighbour counting and advanced table look up otherwise known as "super-decoding";
- **stage (3)** performing the update by comparison of the transition matrix with a random number. The random number generator, G05FAST, consists of a whole set shift registers. The routine is based on the Merzenne prime $2^{7}-1$ which is built into the updating code so that 2 sets of 127 bit planes (bips) are generated by each call to G05FAST. 24 bit unsigned integers are constructed by taking 7 bips from from independent generators from the 2 sets of 127 planes. Some of the bips used at the most significant end are reused as the least significant bips. The use of 24 bips corresponds to specifying $K_{nn}$ to an accuracy $\delta K_{nn}/K_{nn}=0.00000006$ and is preferred to using real numbers where bips are wasted in the exponent when normalising to 1 unless special care is taken. Even with this waste avoided using such real numbers via a real number comparison includes an exponent check which we know need not be made for our normalised numbers. The G05FAST has stood up to thorough 2 d Ising model tests and has produced high statistics for 3 d quantities in agreement with the best estimates of Fisher and Chen's sophisticated series analysis (1986). The nearest neighbour counting has been refined to a minimal set of logical APAL instructions (the basic unit being the add with carry) to obtain the so-called super-decoded planes used to represent the transition matrix in stage 3. In the look up table (table as data) implementation as described in chapter 2 the nearest neighbour counts determine, via some logic (advanced look up), which values to take from the table and load into the appropriate element of the transition matrix. The transition matrix is then compared with a random number matrix, and where greater the spin is flipped. A mask ensures flipping occurs where the nearest sum is -3, -2, -1, 0. In the table as code method loading the transition matrix with probabilities...
looked up in a table followed by testing where transition is greater than random is replaced by writing the transition matrix into the code which performs the transition matrix random number comparison. This can be done where the coupling \( K_{nn} \) is known at compile time. The nearest neighbour count and the corresponding superdecoded bit planes are now tabulated for reference in what follows.

<table>
<thead>
<tr>
<th>trans</th>
<th>nn count</th>
<th>MS</th>
<th>MD</th>
<th>L\text{XOR}(MD and L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \exp(-4K_{nn}) )</td>
<td>4</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( \exp(-8K_{nn}) )</td>
<td>5</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>( \exp(-12K_{nn}) )</td>
<td>6</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

In the case of the 3 d Ising model probabilities: \( p_4 = \exp(-4K_{nn}) \); \( p_5 = \exp(-8K_{nn}) \); \( p_6 = \exp(-12K_{nn}) \) represented as 24 bit unsigned integers if written out as:

\[
\begin{align*}
p_4 &= 000101010110110011010101010
\end{align*}
\]

\[
\begin{align*}
p_5 &= 0000001111011010110000011
\end{align*}
\]

\[
\begin{align*}
p_6 &= 00000000001001011000001
\end{align*}
\]

represent the bit values the transition matrix should have for nearest neighbour (nn) counts of 4, 5 and 6. The key observation is that at each bit significance there are only 8 possible patterns the \( n^{\text{th}} \) bits of \( p_4 \), \( p_5 \) and \( p_6 \) taken together can form. If \( p_4p_5p_6 \) is 111 then the \( n^{\text{th}} \) bit of transition should be true where the count is 4, true where the count is 5 and true where the count is 6. Fetching a .TRUE. plane achieves this. If \( p_4p_5p_6 \) is 110 then the \( n^{\text{th}} \) bit of transition should be 1 where the count is 4, 1 where the count is 5 and 0 where the count is 6. Fetching the inverse of the middle bit of the nearest neighbour count will achieve this. If \( p_4p_5p_6 \) is 101 then the \( n^{\text{th}} \) bit of transition should be 1 where the count is 4, 0 where the count is 5 and 1 where the count is 6. Fetching the inverse of the exclusive or of the middle and least significant bits of the nearest neighbour count achieves this. If \( p_4p_5p_6 \) is 100 then the \( n^{\text{th}} \) bit of transition should be 1 where the count is 4, 0 where the count is 5 and 0 where the count is 6. Fetching the inverse of the
least significant bit of the nearest neighbour count achieves this. There are only 8 patterns formable by p4p5p6 and the remaining patterns are formed using the appropriate superdecode planes not inversed. The superdecode planes required to be fetched to represent the n<sup>th</sup> bit of the transition matrix are given below.

<table>
<thead>
<tr>
<th>p4</th>
<th>p5</th>
<th>p6</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

The transition random number matrix comparison consists of adding with carry the 24 bips which are fetched to represent the transition matrix and the 24 bips of the random number starting at the least significant end. We are only interested in detection of a carry after the 24<sup>th</sup> bips have been added and can discard the resulting less significant bips. Where a carry results at the most significant end then we know transition was greater than or equal to the random number and a spin flip is performed. So far we have only looked after the counts 4, 5 and 6. The other counts 0, 1, 2 and 3 require a spin flip to be performed. The .not. of the MS<sup>bit</sup> where true over rules the carry bit and ensures counts 0, 1, 2 and 3 are always updated.

As it stands this code for 128<sup>3</sup> achieves 219 Mhz (or single spin update attempts per second). The break down of the timings per spin plane update attempt are:

| Neighbour counts plus XOR | 23.1 cycles |
| Random number generation | 24.4 cycles |
| Transition random number comparison | 45 cycles |
| and spin update control overheads | 1 cycle |
| total | 93.5 cycles |

For the DAP a machine cycle takes 1 nanosecond hence the update rate of 219Mhz.
Further speed up

A further saving on the random number generation overheads can be made by loading the DAP with several systems of different size or coupling or even type, and using the same random numbers to update each. The only limit on this is the finite size of the DAP. For the 4096 bips deep DAP at Edinburgh can comfortably lodge 5 128³ systems reducing the random number overheads by 5 to give an 277 Mhz. For smaller systems or for a larger DAP the cost of random numbers per plane update attempt could be reduced to ~ 1 cycle to give 292 Mhz.

A second possibility is to reduce the 24 bit accuracy to 12 bit accuracy but to use several tables as code corresponding to the nearest 12 bit representations which straddle the desired coupling K_{nn} and to simulate calling the different tables with appropriate frequency so as to interpolate to the desired K_{nn}. Reddaway et al refer to this as probability equalisation and it could reduce the random number costs per plane and transition random number comparison by a factor of 2 to give 0.397 Ghz for simultaneous simulation of 5 systems.

Within the table as code structure there remain several small refinements. The transition matrix random number comparison can be made by adding transition and the 2s complement of the random number (or just the random number) or by adding the twos complement of transition and adding to the random number. The former giving a carry where update is to occur the latter carry where update is not to occur. When generating the table as code the comparison can be chosen so as to give as many lines as possible where the null character string (indicating addition of 000) is brought. This, for K_c typically saves 2 cycles out of 45 in the comparison code but for colder systems with smaller Boltzmann probabilities gives increasing savings.

The conjectured maximum for a 12 bit probability equalisation table as code implementation of the Metropolis algorithm on as many 3 d Ising models as fit in the DAP is 0.460 Ghz.

Creutz' Demons for the 3 d Ising model

A demon simulation on the DAP for the 3 d Ising model is considerably faster than the Metropolis algorithm (for a single system simulation) because
no random numbers are required to perform the update. At most 6 random bit planes per 32 sweeps of the system are needed if one wishes to randomly shuffle the 4096 demons in between each update two 6 bit vectors being sufficient to completely shuffle in the north and east directions via north and east shifts of 0±63. The nearest neighbour counting involves adding the number of presently broken nearest neighbour bonds to the present demon to create a trial demon. The update consists of testing whether the trial demon has 0 to nmax quanta in his sack on completion of the addition, update occurring and the trial demon sack contents being assigned to the present demon only where this accommodation test is passed.

Within this implementation the choice nmax determines the update. The effect of nmax on the ensemble averages can be calculated and resulting averages adjusted. We have chosen a 3 bit demon corresponding to a maximum sack contents of 7 quanta of $4K_{nn}$ (the smallest energy change per site for the Ising model). The demon can underflow by 3 quanta or overflow by a maximum of 3 quanta (for the 3 d Ising model) and two 3 bit comparisons must be made to give the following performance.

<table>
<thead>
<tr>
<th>Neighbour counting</th>
<th>Random numbers</th>
<th>accommodation by demons and update control overheads</th>
<th>total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>20 cycles</td>
</tr>
</tbody>
</table>

corresponding to 0.635 G Hz. A 2 bit sack which is the minimum size before limit cycles have to be guarded against, gives 0.718 G Hz.

A 4 coupling improved action is presently being written for which each term in the Hamiltonian has a constraint imposed on it by a demon. Bhanot (1985) has used this method to estimate coupling constants; we intend to perform an improved action MCRG simulation using the couplings calculated in chapter 4. The 4 sets of demons corresponding to the couplings $K_{100}$, $K_{110}$, $K_{111}$ and $K_{200}$ have 3, 4, 4 and 3 bit sacks corresponding to the maximum counts of 6, 12, 8 and 6 associated with the respective neighbour operators. The neighbour counting thus involves 6+12+8+6 broken bonds. The demon accommodation involves 2 comparisons for each demon type where the comparisons are for 3, 4, 4 and 3 bit numbers corresponding to the different
size sacks. The update is performed and the 4 trial demons assigned to the 4 demons where all 4 sack types can accommodate their associated spin operator changes. The expected performance is

<table>
<thead>
<tr>
<th>Task</th>
<th>Cycles</th>
</tr>
</thead>
<tbody>
<tr>
<td>neighbour counting</td>
<td>106.6</td>
</tr>
<tr>
<td>demon accommodations</td>
<td>32</td>
</tr>
<tr>
<td>overheads</td>
<td>1</td>
</tr>
<tr>
<td>total</td>
<td>167.6</td>
</tr>
</tbody>
</table>

corresponding to 0.122 Gzh.

Recently Herman (1986) has performed a microcanonical ensemble simulation which corresponds to a demon with zero sack size (or no demons). He achieved for 2 d Ising models on lattices of $128^2$ up to $1280^2$ an update speed of 0.670 Gzh on a Cray XMP. We have implemented equivalent algorithms on the DAP and obtain an update attempt frequency of 1.75 Gzh for $128^2$. For the 3 d $128^3$ system this number falls in proportion to the increased number of neighbours to give 1.20 Gzh.

The table below indicates the present state of fast algorithms on various supercomputers.

**Metropolis**

<table>
<thead>
<tr>
<th>L</th>
<th>Update Speed</th>
<th>Mhz d=3</th>
<th>Computer</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>L=8..44</td>
<td>93</td>
<td>2 pipe CDC CYBER 205</td>
<td>Bhanot (1986)</td>
<td></td>
</tr>
<tr>
<td>L=8..192</td>
<td>219</td>
<td>ICL DAP</td>
<td>Reddaway <em>et al</em> (1985)</td>
<td></td>
</tr>
</tbody>
</table>

**Demon**

<table>
<thead>
<tr>
<th>L</th>
<th>Update Speed</th>
<th>Mhz d=3</th>
<th>Computer</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>L=8..192</td>
<td>0.635</td>
<td>ICL DAP</td>
<td>Toral and Wall (1986)</td>
<td></td>
</tr>
</tbody>
</table>

**Microcanonical**

<table>
<thead>
<tr>
<th>L</th>
<th>Update Speed</th>
<th>Mhz d=2</th>
<th>Computer</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>L=128..1280</td>
<td>0.670</td>
<td>Cray XMP</td>
<td>Herrmann (1986)</td>
<td></td>
</tr>
<tr>
<td>L=8..128</td>
<td>1.750</td>
<td>ICL DAP</td>
<td>Toral and Wall (1986)</td>
<td></td>
</tr>
</tbody>
</table>
Quality of ensemble averages using fast algorithms

So much for the speed what about the physics produced by the various algorithms in table (5.1). The Edinburgh code with the exception of the improved action is being generalised to all $L=2,4,8,16,32,64,128$ for 2 and 3 d Ising model. This has already been done for the Metropolis algorithm and 3 d work testing the validity of hyperscaling yields the high quality ensemble estimates of chapter 2. The 2 d Metropolis code has been used extensively by Toral and Wall (1986) in a finite size scaling investigation of clusters of spins. The work of Barber et al has tested the IMP fast code for the Metropolis algorithm though their results are not in agreement with the comparable tests of Bhanot on the CDC CYBER who achieves estimates for $\gamma/\nu$ in very good agreement with the work of Fisher and Chen (1985).

The canonical, demon and microcanonical ensembles should give the same ensemble estimates in the infinite volume. In order to decide which algorithm to use for a simulation a knowledge of the equilibration and relaxation times is required together with a knowledge of the fluctuations of the quantity of interest. A comparative study of the fast Metropolis, demon and microcanonical is presently in progress at Edinburgh. For various sizes of lattice ranging from $L=2...128$ the Ising model with periodic boundary conditions for $d=2$ and $d=3$ the equilibration, relaxation times and the fluctuations in the magnetisation and the nearest neighbour energy are being estimated in for control parameters corresponding to criticality. The first indications are that relaxation exponents for the 3 ensembles in $d=2$ systems are the same but the time taken for the magnetisation to change sign, a rough measure of the relaxation time, indicates that the relaxation amplitude is smallest for the Metropolis algorithm gradually increasing to its largest value in the microcanonical ensemble. This is as expected since the energy fluctuations allowed in the Metropolis algorithm allow configuration changes to occur which would be disallowed in the demon and microcanonical ensembles, and hence for greater change in a small number of single spin flips. Thus the faster updating time of the microcanonical ensemble may be of little advantage because it is cancelled by the increased relaxation times. The use of the demon algorithm and particularly the zero sack demon may be useful for Improved action simulations where care is taken to measure local spin operators and ensemble average before averaging over lattice sites.
Particularly the use of Callen's representation here (though its justification is a bit uncertain) might get round the problem of knowing the couplings implicit in the spin configurations produced which for comparison with canonical averages we would like to know.
CONCLUDING REMARKS

In this thesis we have reported the results of a number of simulations of the Ising model on a massively parallel computer, the ICL DAP. The power of the DAP has allowed an extensive simulation to be made on three dimensional lattices of spatial extent \( L = 2, 4, 8, 16, 32, 64 \) and 128. The high statistics obtained and the sophisticated finite size scaling analysis yield no evidence for the violation of hyperscaling and estimates of critical exponents comparable with those obtained by other methods to date. In addition, as explained in chapter 3 coupling constant flow in a MCRG numerical experiment by a two lattice comparison method, confirm the standard picture of flow towards the Ising fixed point in irrelevant directions and away from the Ising fixed point in relevant directions. Our results for exponents obtained by optimised MCRG are not as encouraging as we had hoped, though the potential of the optimisation strategy is not in dispute. Finally, we have developed very fast algorithms for generating spin configurations on a range of lattice sizes for the canonical, demon and microcanonical ensembles. These are allowing a wider range of physics, such as heat flow, to be studied.
REFERENCES


Binder, K., in "Phase Transitions and Critical Phenomena",


Brezin, E., J. C. Le Guillou and J. Zinn-Justin, in vol. 6
"Phase Transitions and Critical Phenomena" C. Domb and M. S. Green,


Burkhardt, Th. W. and J. J. van Leeuwen, "Real Space Renormalisation"


Creutz, M., "Deterministic Ising Dynamics" Brookhaven preprint,

Domb, C. "Phase Transitions and Critical Phenomena" 3 edited by


Halmos, P. R., Lectures on Ergodic Theory, (Chelsa, New York, 1956).


Niemeijer, The. and J. M. J. van Leeuwen, in “Phase Transitions and Critical Phenomena ”, Vol. 6, ed. by C. Domb and M. S. Green


Wilson, K. G. "MCRG and the 3 dimensional Ising model", in Progress in Gauge Field Theories, eds. t Hooft et al. Plenum, (1984).