Finite-Lattice Studies in Hamiltonian Field Theory

A thesis submitted for the degree of Doctor of Philosophy at The Australian National University.

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This dissertation is an account of work carried out while I was enrolled as a student in the Department of Theoretical Physics, Australian National University between March, 1985 and October, 1988 under the supervision of Dr. Christopher Hamer. For the last year of my study I was a 'visiting student' at the Department of Theoretical Physics, University of New South Wales.

As indicated in the text, chapters 1 and 2 are reviews; the appropriate references are given in the text. The remaining chapters, except where indicated, present work which has been done either in collaboration with Dr. Hamer or inspired by him.

None of the work reported here has been submitted to any other institution of learning for any degree.

Christopher Allton

Christopher Allton

7th October, 1988.
Acknowledgements.

I've put off writing this until the very last moment - as will be my way. This is definitely the most read section of a thesis and the hardest to write so I should have put more time into it.

Chris Hamer has been a marvellous friend, instructor, guide and colleague. Never once when I knocked on his door did he say he couldn't give me some time. I thank him for his teaching, warmth and gentle criticism.

My thanks also to the department at ANU for being such homely hosts, especially to Brian and Prof Le Couteur, to my comrade-at-arms Ming, and to one who is truly wasted on physics - Joan.

Many thanks are due to the department at UNSW for treating me as their own, and for being such warm hosts. With ANU close to ski-ing and UNSW close to the beaches (a lunch-time away in fact), I can't complain about my luck.

To the many people who have helped me since March 1985: my (many?) friends, my (many) flatmates, my guitars, family, politicians-to-be, colleagues, those who are nearby and far away ... my dearest appreciation. I won't start thanking you all by name since now it'll force me to do it in a much better way: face-to-face.
Abstract.

An overview is given for the finite-lattice Hamiltonian approach for calculating the critical properties of field theories and statistical mechanics systems. The method is then applied in two main projects to the 2-dimensional O(2) and 3-dimensional Z(2) models.

The overview breaks the method into two halves: (i) the numerical solution of the lowest energy states of finite-lattice Hamiltonians, including schemes to accurately and efficiently truncate unmanageably large Hilbert spaces into tractable subspaces; (ii) the extrapolation of these finite-lattice results to determine the bulk critical behaviour using conformal invariance and finite-size scaling techniques. An example of the above approach is given in a study of the lattice harmonic oscillator.

In the first main project, the (1+1) dimensional O(2) or planar rotator model is examined in detail using the Hamiltonian finite-lattice approach. The critical point is found to be $x_c \approx 2.0$, leading to the conjecture $x_c = 2$, the conformal anomaly $c$ is confirmed to be unity, the correlation length exponent $\sigma$ is given by $\sigma = 0.50$ agreeing with the Kosterlitz prediction $\sigma = 1/2$, and the exponent $\eta$ is found as a function of coupling. The O(2) invariant partition function studied by Nienhuis, Baxter, Batchelor and Blöte is shown to have the same Hamiltonian form as the canonical model.

In the second project, a new Monte Carlo style truncation scheme for the Hilbert space, 'stochastic truncation', is tested on the (2+1)-dimensional Z(2) gauge model. This method gives accurate results, free from systematic errors, but only when a large amount of computing power is invested so that the statistical errors are small.
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Chapter 1
Introduction

"I think that I had more or less given up on my thesis. Even now that I have resumed work it is not with great confidence in what I am producing."

Senior Lecturer in Law, University of Witwatersrand,
United Democratic Front member,
Political Detainee without trial - South Africa.

§1.1 A Description of the Problem.

In many areas of physics there is a fundamental problem of finding a system's lowest energy states. For fields as diverse as statistical mechanics, molecular and elementary particle physics it is essential to know the preferred states of a system in order to predict its behaviour. This dissertation outlines the study of systems with many degrees of freedom by calculating their preferred states using a quantum field theory/statistical mechanics formalism.

For quantum field theories, information about the ground and low lying excited states of the Hamiltonian leads to vacuum properties of the system (eg. propagators) and details of the massive spectrum (eg. allowed bound states and their masses).
In Lagrangian (conventional) statistical mechanics, the lowest energy state is the equilibrium one which corresponds to the greatest eigenvalue of the transfer matrix. This eigenvalue can be used to define the free energy which in turn determines the position and nature of any critical point in the system. All thermodynamic functions can be expressed in terms of the free energy so the critical exponents can also be found from the equilibrium's transfer matrix eigenvalue. This statistical mechanics approach is shown in the next section to be entirely equivalent to a quantum field theory formulation, so both fields can be effectively treated as one.

The principle aim of this dissertation is to study the behaviour of some field theory/statistical mechanics models by developing techniques to find their lowest energy states and thus uncover the wealth of information about the systems described above. Specifically the systems of interest are lattice gauge models and spin systems. For a review of this area of physics see Kogut (1979). The various methods used in the study of this field are outlined in §1.3.

§1.2 Quantum Field Theory, Statistical Mechanics and Lattice Gauge Theory.

In the last couple of decades it has become apparent that statistical mechanics and field theory are really two different physical formulations of the same mathematics. This is easily seen at a very fundamental level (Kogut 1979, Hamer 1988). The basic quantity is statistical mechanics is the partition function
\[ Z_{SM} = \prod_{\text{sites}} \sum_{\sigma(j)} \exp \left( -\mathcal{H}(\sigma(j)) / k_B T \right) \]  

(1.1)

where the sum is over all possible values of \( \sigma(j) \) which represents the degree of freedom at site \( j \), \( \mathcal{H} \) is the energy function or classical Hamiltonian of the system, \( k_B \) is the Boltzmann constant and \( T \) is the temperature.

A fundamental quantity in quantum field theory is the path integral

\[ Z_{QFT} = \lim_{a, \Delta t \to 0} \left\{ \prod_{j=(x,t)} \int d\Phi(j) \right\} \exp \left( i \frac{S(\Phi(j))}{\hbar} \right) \]  

(1.2)

where the field \( \phi(j) \) is defined on a discrete lattice with spacings \( a \) and \( \Delta t \) in the spatial and time directions and the (classical) action of the system is \( S \). The limit \( a, \Delta t \to 0 \) recovers the continuum theory.

Now if we were only interested in a field theory on a lattice then our path integral would be

\[ Z_{\text{lattice QFT}} = \left\{ \prod_{j=(x,t)} \int d\Phi(j) \right\} \exp \left( i \frac{S(\Phi(j))}{\hbar} \right) \]  

(1.3)

The mathematical equivalence of (1.1) and (1.3) is immediately apparent, that is

\[ Z_{\text{lattice QFT}} = Z_{SM} \]  

(1.4)

This is strictly true only after a 'Wick rotation' in which the Minkowski space of (1.3) is transformed into the Euclidean space of (1.1) (this removes the factor of \( i \) in the exponent of (1.3)).

Thus statistical mechanics can be said to be the study of discrete versions of field theories. Equally field theory can be solved in a 'statistical mechanical' formulation on a discrete lattice with the physical answers
obtained by letting the lattice spacings go to zero at the end of the
calculation. These various formulations of field theory/statistical
mechanics and their relationships are shown in figure 1.1. It is worth
pointing out at this stage that the critical behaviour (ie. the type of any
phase transition and the values of the critical indices) is the same for all
formulations whether lattice or continuum, Minkowski or Euclidean.
This follows from the principle of universality.

<table>
<thead>
<tr>
<th>CONTINUUM</th>
<th>EUCLIDEAN</th>
<th>MINKOWSKI</th>
</tr>
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<tr>
<td>Discretize</td>
<td></td>
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<td>LATTICE</td>
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**Figure 1.1** Quantum Field Theory, Statistical Mechanics and the relationships between them.

From the equivalence between $Z_{SM}$ and $Z_{lattice \ QFT}$ other correspondences between statistical mechanics and field theory quantities follow.
These are listed in table 1.1.

<table>
<thead>
<tr>
<th>STATISTICAL MECHANICS</th>
<th>QUANTUM FIELD THEORY</th>
</tr>
</thead>
<tbody>
<tr>
<td>(d spatial dimensions)</td>
<td>(1 time and d-1 spatial dimensions)</td>
</tr>
<tr>
<td><strong>Partition Function</strong></td>
<td><strong>Path Integral</strong></td>
</tr>
<tr>
<td>$Z_{SM}$</td>
<td>$Z_{QFT}$</td>
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<tr>
<td><strong>Spins</strong></td>
<td><strong>Fields</strong></td>
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<tr>
<td>$\sigma(l)$</td>
<td>$\phi(r)$</td>
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<tr>
<td><strong>Equilibrium State</strong></td>
<td><strong>Ground State</strong></td>
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<tr>
<td><strong>Classical Hamiltonian</strong></td>
<td><strong>Action</strong></td>
</tr>
<tr>
<td>$-\mathcal{H}$</td>
<td>$S$</td>
</tr>
<tr>
<td><strong>Log Transfer Matrix</strong></td>
<td><strong>Hamiltonian</strong></td>
</tr>
<tr>
<td>$-\ln V$</td>
<td>$i\mathcal{H}$</td>
</tr>
<tr>
<td><strong>Free Energy</strong></td>
<td><strong>Ground State Energy</strong></td>
</tr>
<tr>
<td>$-F$</td>
<td>$\omega_0$</td>
</tr>
<tr>
<td><strong>Correlation Function</strong></td>
<td><strong>Propagator</strong></td>
</tr>
<tr>
<td>$\exp(-r/\xi)$</td>
<td>$\exp(-\mu r)$</td>
</tr>
<tr>
<td><strong>Correlation Length</strong></td>
<td><strong>Inverse Mass Gap</strong></td>
</tr>
<tr>
<td>$\xi$</td>
<td>$1/\mu$</td>
</tr>
<tr>
<td><strong>Soliton</strong></td>
<td><strong>Instanton</strong></td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td><strong>Coupling</strong></td>
</tr>
<tr>
<td>$T$</td>
<td>$g$</td>
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**Table 1.1** Correspondences between Statistical Mechanics and Field Theory.

The realization of the equivalence of statistical mechanics and field theory has helped the evolution of lattice gauge theory which effectively straddles the two fields.

Lattice gauge theory was formulated by Wilson (1974) as a mechanism for describing the confinement of quarks using gauge fields and a lattice to act as an ultraviolet cut-off. Important further developments have been made by Kogut and Susskind (1975) and Fradkin and Susskind (1978). Kogut (1979) has reviewed the field with emphasis on its similarities with statistical mechanics.

In lattice gauge theory many of the vast array of statistical mechanics methods are used to solve gauge field theories. The ultimate
aim is to make predictions from the theory of quark interactions - quantum chromodynamics. The language used in lattice gauge theory (and in this dissertation) is a mixture of both field theory and statistical mechanics terminology as lattice field theorists make no distinction between the two fields. (Table 1.1 provides a translation where necessary.)

One particularly important feature of lattice gauge theory as a method of solving field theories is the role of the correlation length. When measured in physical units this can be written

\[ \xi_{\text{physical}} = n_\xi a \]  

(1.5)

where \( n_\xi \) is the number of lattice sites corresponding with the correlation length. To relate this to a non-trivial field theory we must have \( \xi_{\text{physical}} \) finite, corresponding with an interacting field theory with a finite mass gap (see table 1.1). This implies that as the lattice spacings go to zero recovering the continuum theory, \( n_\xi \) must diverge, signalling a critical point. So the (non-trivial) continuum limit corresponds to the critical point of the lattice system.

This presents a stumbling block for progress in lattice field theories because critical systems, due to their singular nature, are fundamentally difficult to study. This problem occurs no matter what approach is taken to lattice gauge theory. For example in the Monte Carlo approach 'critical slowing down' lengthens the equilibration time of the simulation, and in the finite-lattice Hamiltonian approach a large number of basis states are required to accurately distinguish between the converging low lying eigenstates at the pseudo-critical point. This last problem is taken up in chapter 3.
§1.3 Summary of Methods Used.

Having described the basics of the problem and the language in which it is formulated, we turn to its solution.

There have been a huge number of methods applied to the study of field theory and statistical mechanics systems. These can be categorized according to the scheme in figure 1.2.

The most obvious (and desirable!) method is the exact solution. Unfortunately very few systems can be exactly solved; even statistical mechanics models as conceptually simple as the three dimensional Ising model remain unsolved (see Baxter 1982), and there are virtually no exact solutions to useful field theories.

\[
\begin{array}{l}
\text{EXACT} \\
\text{APPROXIMATE ANALYTIC} \\
\quad \text{- PERTURBATION EXPANSIONS} \\
\quad \text{- RENORMALIZATION GROUP - 'Direct'} \\
\quad \quad \text{- } \varepsilon \text{ expansions} \\
\quad \quad \text{- } 1/n \text{ expansions} \\
\quad \text{- VARIATIONAL} \\
\quad \text{- SPECIAL/ MODEL DEPENDENT} \\
\quad \text{NUMERICAL} \\
\quad \text{- MONTE CARLO - Euclidean} \\
\quad \quad \text{- Hamiltonian} \\
\quad \quad \text{- Renormalization Group} \\
\quad \text{- 'EXACT' FINITE-LATTICE HAMILTONIAN}
\end{array}
\]

Figure 1.2 Methods of Solution of Quantum Field Theory/Statistical Mechanics Problems.
There are many models for which no exact solutions have been found, but which have approximate analytical solutions. There are a huge variety of methods used to obtain these approximate solutions but (leaving aside mean-field approaches) they fall into four general classes:

(i) Those using a perturbation style expansion. These involve a series in the coupling or temperature parameter, usually expanded about the T=0 or T=∞ point in phase space. Usually an appropriate thermodynamic quantity, often the partition function, is expanded into a series involving graphs of flipped spin (say), of higher and higher topological complexity. Equivalently a Rayleigh-Schrodinger expansion may be obtained from the system’s Hamiltonian. The series expansion method has proved extremely useful for a number of models and has reached a level of sophistication where some exact predictions of critical quantities have been made. (See Guttmann 1988 for a review.)

There are two main problems with the perturbation expansion method. The first is computational: the time taken to calculate the nth term grows exponentially with n. This typically means that the time taken to calculate the (n+1)th term is greater than the total time taken to calculate the first n terms. The second problem is mathematical: by definition the series obtained is analytic and therefore cannot directly reproduce the singular nature of a critical point. Various analytical methods have had to be developed to extrapolate to the singular behaviour.

(ii) Those involving a renormalization group argument. The renormalization group treatment enables one to deal with field theories and critical lattice systems which have fluctuations on all length scales...
and therefore do not possess a characteristic interaction length. (See eg. Barber 1977, Domb and Green 1976, Fisher 1983)

There are three analytic renormalization group approaches. The first follows the Kadanoff-Wilson scheme directly by solving the problem interatively at a number of nested length scales. The final solution then includes contributions of every length scale in the system.

The second method involves the ‘ε-expansion’. It was noted by Wilson and Fisher (1972) that a perturbation style approach is feasible if one used the expansion parameter \( \varepsilon = 4-d \), where \( d \) is the dimensionality of the system. This is a ‘natural’ parameter to use since the results of mean field theory hold at four dimensions and above. This expansion can be used in the critical region itself and it gives estimates of the critical exponents as a series in \( \varepsilon \).

The third renormalization group technique is the 1/n expansion (Abe 1972) where \( n \) is the dimensionality of the degrees of freedom (spins) in the system. This method is effectively an expansion about the (soluble) spherical model which corresponds to \( n = \infty \).

The renormalization group is an important and novel approach to the subject, but the expansion methods suffer from the problem of rapidly growing complexity at each order and thus far the critical exponents have been calculated to fourth order only.

(iii) Those using a variational approach. The basic idea here is to 'guess' a form \( |\psi(\alpha)\rangle \) for the ground state of a Hamiltonian \( H \) involving the parameters \( \{\alpha\} \). The estimate of the ground state energy (which is always an upper bound) is given by
\[ \omega_0 = \min_{\{\alpha\}} \frac{\langle \psi(\alpha) | H | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle} \]  

(1.6)

where the minimum is over the parameter space of \( \{\alpha\} \). Obviously the choice of the wave function \(|\psi(\alpha)\rangle\) is critical; there is no use estimating the weak coupling behaviour with a strong coupling ansatz. There are a number of improvements that can be made to the above scheme, an obvious one being to use a more complicated form for \(|\psi(\alpha)\rangle\) involving more parameters. Another improvement is to invoke the Lanczos scheme (see §3.3) to create a sub-space including \(|\psi(\alpha)\rangle\) in which a better estimate of the ground state and energy may be found.

There have been many papers applying the variational technique to field theories (see eg. Horn and Weinstein 1982, Dagotto and Moreo 1985, Heys and Stump 1987, Choe et al 1988 and references therein) with some indication that there may be future success in quantum chromodynamics calculations.

The difficulties with the method concern the computational complexity of calculating the necessary matrix elements (cf. (1.6)) and the choice of a physically appropriate ansatz \(|\psi(\alpha)\rangle\) which correctly maps the complex structure of the true ground state.

(iv) The last approximate analytic method uses special or 'trick' techniques which rely on known features of individual models. A classic example of this is Kosterlitz and Thouless' work on the two dimensional O(2) or x-y planar model (Kosterlitz and Thouless 1973). The special feature they used was the presence of 'vortices' in the model. They expanded the partition function into a vortex contribution and a background spin-wave component and were able to predict the precise
nature of the model’s phase transition and an approximate value for the
critical point. The obvious difficulty with this approach is that these sorts
of special features in a model cannot generally be found and utilized.

The third main approach to the solution of quantum field theory and
statistical mechanics problems uses numerical techniques (see figure 1.2).
By far the most popular numerical treatment involves the ‘Monte Carlo’
(MC) approach, so it will receive a deal of attention here.

It is convenient to divide the various MC schemes into three
reasonably separate approaches:-

(i) Euclidean MC. This is the main method used at present for the
numerical calculation of phase transitions and lattice gauge theories. It
is best described using statistical mechanics language (see the previous
section for the field theory equivalent - especially figure 1.1). The aim of
the Euclidean MC treatment is to make a direct numerical calculation of
the finite-lattice partition function by generating a set of configurations \( \{ \phi \} \)
which is characteristic of the full ensemble. The configurations are
generated by the Metropolis, heat bath, molecular dynamics
(microcanonical), or Langevin algorithms, or by a 'hybrid' of them. The
best algorithm seems to depend on the system being studied. For brevity's
sake the algorithms for generating the ensemble will not be discussed
here.

Once the configuration set has been generated it is easy to calculate
an approximation to any physical quantity \( \Omega \) simply by the formula

\[
\langle \Omega \rangle = \frac{1}{N_\Phi} \sum_{\{\phi\}} \langle \phi \mid \Omega \mid \phi \rangle
\]

(1.7)
where $N_\phi$ is the number of configurations in $\{\phi\}$. The number of times a configuration $\phi$ appears in the set $\{\phi\}$ will be proportional to its Boltzmann weight. For a review of the Euclidean MC method see for example Creutz et al (1983), Kalos (1984), Binder (1987).

(ii) Hamiltonian MC. This method is similar in spirit to the Euclidean approach in that a representative configuration set is formed, but in this case the configurations are elements of the Hilbert state space appropriate to the Hamiltonian of the system. Its main advantage over the Euclidean formalism is that its configurations have one less spatial dimension - see §1.2. In the standard formalism a configuration set is generated at time $t_{n+1}$ from the configuration set at time $t_n$ by the application of the Hamiltonian (which is the time translation generator). In the case of 'projector MC' (see Blankenbecler and Sugar 1983) this ensemble set only contains a single state, but the 'ensemble projector MC' method's ensemble set contains many states (see De Grand and Potvin 1985).

A new Hamiltonian MC method has been proposed (Hamer 1987) which provides a natural means of treating only the 'most significant' states in the full Hilbert space. This method is used in a project in chapter 5 and will be discussed more fully there.

Both the Euclidean and Hamiltonian MC methods have their accuracy determined by the memory capacity and processing speed of present computers. There is for example a limit on the lattice sizes that can be studied (up to the order of $10^4$ lattice sites) which is small considering that the bulk behaviour has to be obtained from these lattices. There is also an obvious limit on the number of time steps or iterations
able to be performed which directly places a lower bound on the statistical errors in the calculation. 'Critical slowing down', where the approach to equilibrium in the critical region is slowed, is also a problem because it may mean that a large amount of the data is 'non-equilibrium' and therefore of no use for non-dynamical studies.

(iii) The last class of MC methods is the Monte Carlo Renormalization Group (MCRG). This is considered here as a numerical method (rather than an approximate analytic approach) since computers are intrinsic to its operation. In this approach a finite-lattice is analyzed with a Hamiltonian involving as many different types of interactions as possible - eg. nearest neighbour, next-nearest neighbour, four-spin etc. A configuration set is generated for this lattice using conventional Euclidean MC and the spins in these configurations are averaged over a block of size b. The blocked system has the same symmetries as the original one but with different interaction strengths (which can be numerically calculated). After a number of such 'blockings' these couplings tend towards the 'fixed point' values and the critical exponents can be found. (See Wilson 1984 for a review.)

There are the usual computational limitations on the MCRG: finiteness of the lattice, statistical errors and the finite number of interaction types that are included (a full analysis would include all possible interaction types!). See Gupta (1986) for a discussion of some more technical problems.

The second numerical method used after MC is the 'exact' finite-lattice Hamiltonian approach (Hamer and Barber 1981a,b). This method represents the finite-lattice Hamiltonian on an appropriate basis and
solves for the ground and low lying excited states using a matrix eigen-
equation. The finite-lattice data are extrapolated to the bulk limit by the
finite-size scaling technique.

For the models whose finite-lattice Hilbert spaces are finite
dimensional exact solutions can be obtained (for small enough lattices).
In the case of models which have infinite-dimensional finite-lattice Hilbert
spaces accurate eigensolutions can be obtained by applying cut-offs to the
basis set.

The method of eigensolving the finite-lattice Hamiltonian is described
in chapter 3 and the finite-size scaling technique is described in §2.3. The
'exact' finite-lattice Hamiltonian approach is taken on a project described
in chapter 4.

The main drawback in this method is again due to limited computer
resources: the lattice sizes that can be solved accurately are even smaller
than those which can be dealt with using the Monte Carlo technique. This
means the bulk behaviour is extrapolated from a very short sequence of
data corresponding to a handful of lattice sizes. 'Short', accurate finite-
lattice data is characteristic of the 'exact' Hamiltonian approach
compared with 'longer', less accurate sequences in the Monte Carlo case.

The main advantage of both numerical methods is that they provide
'direct' solutions to the problem - they are valid in principle for all values
of the coupling parameter. So unlike perturbation series expansions the
critical region poses no barrier to the investigation of the system's entire
phase diagram. (In practice, the accuracy of the solutions is poor when
the coupling involved becomes large.)
§1.4 Brief Description of the Models Studied and Approach Taken.

This section briefly overviews the two main projects that make up this dissertation. They are the study of the (1+1)D O(2) or x-y planar model and the (2+1)D Z(2) gauge models using finite-lattice Hamiltonian methods (Hamer and Barber 1981a,b).

There are several reasons to choose these models. the (1+1)D O(2) model has a non-typical phase structure; it has a standard high-temperature region and a low temperature region with infinite correlation length but with zero spontaneous magnetization (ie. no long range order). This contrasts strongly with standard first and second order phase transitions. It has also been shown (Migdal 1975) that the two dimensional O(2) model is related to the four dimensional U(1) model in that they both have similar renormalization group equations.

The (2+1)D Z(2) model is interesting for several reasons as well. It is 'dual' with the 3D Ising model (see §V.E Kogut 1979); its high (low) temperature region corresponds with the 3D Ising model's low (high) temperature phase. It is also the simplest gauge model possible.

Thus both models are interesting in their own right as a study of phase transitions and critical phenomena, and because they are related to other significant physical models. As well as this they can be seen as test-bed models where techniques can be used with a view to application on four dimensional lattice gauge theories. One couldn't imagine any technique being successful on a four dimensional lattice gauge system if it weren't applicable to these two simpler systems. The models also contrast with each other in that the O(2) system has an infinite number of states per site whereas the Z(2) model has only a finite number. Also the O(2)
model has \textit{global} $O(2)$ symmetry whereas the $Z(2)$ has \textit{local} (gauge) symmetry.

The numerical study of both models involves solving the lowest energy states of the system's (quantum) Hamiltonian. As described in §1.1 this leads to a wealth of information, including the position and nature of the phase transition, the values of the critical exponents, and thermodynamic and physical quantities like the magnetization and string tension.

In the $O(2)$ chain, the 'exact' finite-lattice Hamiltonian method is applied. Solutions on the finite-lattice are obtained by representing the Hamiltonian on 'strong coupling' basis states and solving for the lowest eigenvalues and their eigenvectors using a generalized Lanczos algorithm. The finite-lattice Hilbert space is infinite, so to make the problem finite a 'naive' truncation scheme is used to throw away states. A method that takes some account of the states which would otherwise be ignored is also tested. These finite-lattice solutions are extrapolated to the bulk limit by finite-size scaling and conformal invariance (see §2.4), leading to values for the critical point, critical indices and the conformal anomaly. The $O(2)$ project is fully described in chapter 4.

In the (2+1)D $Z(2)$ case obtained using a Monte Carlo finite-lattice Hamiltonian method known as 'stochastic truncation'. This new technique is an iterative method of stochastically choosing a sample of basis states and their weights to represent the eigenvector. Thus quantities derived from this method are averaged quantities and have statistical errors associated with them. The $Z(2)$ project is presented in chapter 5.
§1.5 Layout of the Thesis

Before the specifics of the O(2) and Z(2) projects are discussed there are two chapters describing the background of the finite-lattice Hamiltonian approach to the study of spin and gauge systems.

Chapter 2 reviews finite-size scaling and conformal invariance. Finite-size scaling is the means by which the bulk behaviour of the model is extracted from finite-lattice results. It is based on the hypothesis of scale invariance; a critical system is invariant under a scale transformation. Conformal invariance is a recent addition to the armoury of techniques available to study two dimensional systems. It is based on the hypothesis that systems at criticality are invariant under conformal transformations. In summary, chapter 2 details the techniques used to work the raw finite-lattice solutions into the bulk behaviour of the system. Obviously before finite-size scaling and conformal invariance can be applied to the problem the actual finite-lattice solutions must be found.

Chapter 3 discusses the techniques of truncating the Hilbert space into manageable portions and illustrates them on the lattice version of the harmonic oscillator. It outlines the various algorithms available to eigensolve the Hamiltonian matrix and details the methods used in the O(2) and Z(2) projects. In summary chapter 3 outlines the stage in the finite-lattice Hamiltonian approach which obtains the finite-lattice solutions from the system's Hamiltonian.

As mentioned in §1.4, chapters 4 and 5 discuss in detail the O(2) and Z(2) projects. Chapter 6 summarizes the results and the methods and proposes some possible future research directions.
Chapter 2

Finite-Size Scaling and Conformal Invariance

"The closest I ever came to seeing things the way the Physicists say things really are,
Was out on Sudbury Marsh one summer eve when a silhouetted tree against the sun,
Seemed at my sudden glance to be a fire, a black and boiling smoke made all its shape,
Binoculars resolved the ensiphered sight to make it clear the smoke was a cloud of gnats,
Their millions doing such a steady dance as by the motion of the many made the one shape constant,
And kept it so in both the forms I thought to see,
The Fire and The Tree.
Strike through the mask you find another mask,
Mirroring mirrors by analogue make visible,
I watched 'till the greatest smoke of night engulfed the other,
Standing out on the marsh amid a hundred hidden streams meandering down from concord to the sea."

- Howard Nimrod.

§2.1 Introduction.

This chapter introduces the important tools of finite-size scaling and conformal invariance and gives a summary of the derivations of the formulae used in both theories. These derivations will not involve mathematically rigorous argument, reference to the original papers will be given for that, but they will give a summary of the steps involved in the full derivation. The aim of this chapter is to present the equations that relate the (bulk) critical behaviour with the finite lattice data, giving some idea of how they can be derived. These equations are to be used later in the second half of the analysis where the bulk behaviour is obtained from the finite-lattice solutions, the first half being the determination of the finite-lattice solutions.
Before delving separately into finite-size scaling and conformal invariance it is worth comparing them. There are some major similarities between them:

(i) They are both based on the hypothesis that the physics of a system at criticality is invariant under a particular transformation of its coordinates. The transformation on which finite-size scaling is based is a \textit{global} dilatation, translation and rotation. In the conformal invariance case\(^\dagger\) it is a conformal transformation of its coordinates, i.e. a \textit{local} dilatation, translation and rotation. Conformal invariance is then a generalization of scale invariance.

Strictly speaking both invariances apply only to continuum models, but when the model is critical the correlation length is infinite, so the coarseness of the lattice is essentially invisible. In both cases the invariances are not proven in general for lattice models\(^\ddagger\), but their predictions agree with the observed behaviour for a large number of systems and have been verified for exactly soluble models such as the Ising model. Thus the scale and conformal invariance hypotheses are elevated to the status of ‘principles’.

One further qualification is that when the system is described as being ‘invariant’ under these transformations what is meant is that the microscopic state’s probabilities are not changed, but, as will be shown later, the correlation functions transform covariantly (see Cardy 1987a).

\(^\dagger\)Unfortunately conformal invariance is the name used for both the type of transformation invariance and the theory derived from the invariance.

\(^\ddagger\)For continuum field theory models it has been shown that both scale invariance (Polyakov 1968, Migdal 1968) and conformal invariance (Polyakov 1970) hold at the critical point.
The second common factor in the theories is that the invariances are used to constrain the behaviour of the critical system. Thus finite-size scaling predicts that, for example, the singular part of the free energy density is a generalized homogeneous function in the neighbourhood of the critical point (Privman and Fisher 1984) and conformal invariance predicts that, for example, the dimensions of certain scaling operators can take only discrete values (Friedan et al 1984).

Thirdly, both theories use the framework (formally at least) of the renormalization group. The results of the renormalization group will be used in later sections in the ‘derivation’ of the equations in both theories.

Finally, and for our applications most importantly, both give a means of extracting the bulk behaviour of the system from its finite-lattice behaviour.

The main difference between finite-size scaling and conformal invariance is that finite-size scaling is applicable to systems of any dimension, whereas conformal invariance provides useful results only in two dimensions. This is because conformal transformations form a group which has infinite dimensions only in two coordinate dimensions. For this reason conformal invariance is applied only to the $(1+1)D$ $O(2)$ model (chapter 4), whereas finite-size scaling is used in the analysis of both the $(1+1)D$ $O(2)$ model and the $(2+1)D$ $Z(2)$ model (chapter 5).

The next section describes a derivation of the equation that determines how correlation functions transform under the renormalization group. Both the sections on finite-size scaling and conformal invariance (§§2.3, 2.4) use this transformation equation to ‘derive’ their results. Section 2.3 presents the finite-size scaling equations
and derives the scaling behaviour of thermodynamic quantities and §2.4 presents an overview of the development of conformal invariance, concluding with Cardy's work on the strip geometry.

§2.2 Transformation Laws for Multi-Point Correlation Functions.

This section outlines the derivation of the transformation law for multi-point correlation functions at the critical point under a renormalization group (RG) transformation. This transformation law will be used in the next two sections to develop the theories of finite-size scaling and conformal invariance. The derivation below is similar in style to that in §2 of Barber's review (Barber 1977), except that the presentation here is based on a real space rather than momentum space cut-off.

Let us begin by defining the statistical mechanics (classical) Hamiltonian for the system of interest to be $\mathcal{H}(s(\mathbf{r}))$, where $\mathbf{r}$ is the position vector on a $d$-dimensional lattice with spacing $\alpha$ and a one component spin $s(\mathbf{r})$ represents the degree of freedom at site $\mathbf{r}$. The system has the usual Boltzmann probability factor of occupying the configuration state $\{s(\mathbf{r})\}$ of

$$P\{s(\mathbf{r})\} = C \exp\left[-\beta_B \mathcal{H}(s(\mathbf{r}))\right] \quad (2.1)$$

where $\beta_B = (k_B T)^{-1}$, $T$ is the temperature and $C$ is an appropriate normalization constant. Multi-point correlation functions of the spin variables are of the form

$$\langle s(\mathbf{r}_1) s(\mathbf{r}_2) \ldots \rangle_{\mathcal{H}} \quad (2.2)$$

where $\langle \ldots \rangle_{\mathcal{H}}$ is the usual ensemble average taken with respect to the probability distribution (2.1).
The aim of the RG is to study the system’s critical region where the long range effects are dominant, the correlation length is large and we are free to average out small distance effects with asymptotic immunity. We can define a RG transformation $R_b$ by the following three steps.

(i) Following Kadanoff’s cell approach we can average over blocks of spin with a linear dimension of $ba$, ($b > 1$), without changing the large scale appearance of the system (ie. the correlation functions for large separations won’t change under this step). This averaging is done in such a way that the averaged spins are elements of the same symmetry group as the original spins. The scale factor $b$ must satisfy $ba << \xi(T)$ or else the physically significant length scales will be removed. This idea of integrating out degrees of freedom is central to the RG approach.

(ii) The system’s coordinates are rescaled $r \rightarrow r/b$, so the spacing between the blocks is the same as the original lattice spacing $a$. (In the momentum space approach this means that the momentum cut-off is the same in both systems.)

These first two steps define a ‘classical’ scale transformation (ie. one which ignores fluctuations).

(iii) To complete the definition of $R_b$ the spin components are renormalized by a constant factor $\rho_b$ and the resulting spins are defined $s'(a)$.

The three steps of the RG transformation $R_b$ are schematically displayed in figure 2.1.

There are many results that can be drawn out of the RG, but we will concentrate on the effect $R_b$ has on the correlation functions. By applying steps (i), (ii) and (iii) to the two-point correlation function we obtain
\[ \langle s(i_1) s(i_2) \rangle_{\mathcal{H}} = \rho_{b}^{-2} \langle s'(\alpha_1) s'(\alpha_2) \rangle_{\mathcal{H'}} \]  \hspace{1cm} (2.3)

We can constrain the form of \( \rho_{b} \) by noting from the steps (i), (ii) and (iii) that we must have

\[ \mathcal{R}_{b} \mathcal{R}_{b'} = \mathcal{R}_{bb'} \]  \hspace{1cm} (2.4)

This, together with (2.3) implies

\[ \rho_{b} \rho_{b'} = \rho_{bb'} \]  \hspace{1cm} (2.5)

which restricts the form of \( \rho_{b} \) to (Aczél 1966,1969)

\[ \rho_{b} = b^{x} \]  \hspace{1cm} (2.6)

for some \( x \). Thus (2.3) can be rewritten

\[ \langle s(i_1) s(i_2) \rangle_{\mathcal{H}} = b^{-2x} \langle s'(\alpha_1) s'(\alpha_2) \rangle_{\mathcal{H'}} \]  \hspace{1cm} (2.7)

---

**Figure 2.1** Representation of the three steps that define the RG transformation \( \mathcal{R}_{b} \).
The index $x$ is called the scaling dimension corresponding to the spin $s(r)$ which in the RG language becomes an operator $\hat{s}(r)$. In general there are many different operators $\hat{\phi}_i$ which are involved with the renormalization of a particular system, each having a corresponding scaling dimension $x_i$. (To understand how these different operators arise it is necessary to study fixed point Hamiltonians and their universality classes. See the review by Barber 1977.) Correlation functions of any of these operators can be found and a simple generalization of (2.7) gives

$$\langle \Phi_1(r_1) \Phi_2(r_2) ... \rangle_{\mathcal{H}} = \prod_j b^{-x_j} \langle \Phi_1'(r_1') \Phi_2'(r_2') ... \rangle_{\mathcal{H}'}$$

(2.8)

where the dashes refer to the new system and the hats on the operators are removed for convenience.

Equation (2.8) thus relates the generalized multi-point correlation functions of the two systems. Our aim is to get a relation involving the correlation functions of the same system. We can do this by firstly studying the Hamiltonians of the two systems. There are two important operators which appear in canonical Hamiltonians: the energy operator $\Phi_E$, and the magnetic or symmetry breaking operator $\Phi_h$. The fields conjugate to these operators are the (reduced) temperature $t$ and the magnetic field $h$. The canonical Hamiltonian is terms of these fields and operators can be written

$$\mathcal{H}(t,h) = t \sum_{\text{sites } \vec{r}} \Phi_E(\vec{r}) + h \sum_{\text{sites } \vec{r}} \Phi_h(\vec{r})$$

(2.9)

By making the cells explicit in the sums over the sites and using the definition of $\mathcal{R}_b$ (see figure 2.1) we get
\[ \sum_{\text{sites } r} \Phi_{\alpha}(r) = \sum_{\text{cells } \alpha} \sum_{\text{sites } r \text{ within } \alpha} \Phi_{\alpha}(r) = b^d \sum_{\text{cells } \alpha} \langle \Phi_{\alpha}(r) \rangle_{\tau = \alpha} = b^{d-1} \sum_{\text{cells } \alpha} \Phi_{\alpha}'(\alpha) \]  

(2.10)

so we obtain
\[ \mathcal{H}(t', h') = \mathcal{H}_b \mathcal{H}(t, h) = \mathcal{H}(b^{y_{t', h'}} t, b^{y_{t', h'}} h) \]  

(2.11)

where \( y_i = d - x_i \).

(2.12)

Importantly, the form of the Hamiltonian is unchanged under a RG transformation and the fields \( t \) and \( h \) are renormalized. Also we know from step (i) that the new system's degrees of freedom, \( s'(\alpha) \), have the same symmetries as the original ones, \( s(\alpha) \). From these facts we can conclude that the new system is precisely the same as the original one, except that it is at a different point in \((t, h)\) space. Equation (2.8) can be rewritten giving the desired result
\[ \langle \Phi_{\tau_1} \Phi_{\tau_2} \cdots \rangle_{\mathcal{H}(t, h)} = b^{x_{y_{t, h}}} \langle \Phi_{\tau_1} b^{x_{y_{t, h}}} \Phi_{\tau_2} b^{x_{y_{t, h}}} \cdots \rangle_{\mathcal{H}(b^{y_{t, h}} t, b^{y_{t, h}} h)} \]  

(2.13)

It should be emphasized that this result is true only in the neighbourhood of the critical point. The following two sections will use (2.13) in their 'derivations' of finite-size scaling (§2.3.2) and conformal invariance (§2.4.1).

§2.3 Finite-Size Scaling.

The systems we will solve numerically have local interactions and are infinite in only one direction - the 'time-like' dimension. (They are finite in the spatial dimensions.) It is known that such systems cannot undergo a phase transition, so they can have no singularities in their free energies. How then is the critical behaviour (critical temperature and
exponents) determined from such non-singular systems? Finite-size scaling can provide the necessary connection between the properties of the finite system and infinite system.

The finite-size scaling equations used in chapters 4 and 5 are listed in §2.3.1 without derivation. Section 2.3.2 'derives' the fundamental finite-size scaling equation from the transformation equation for the correlation functions (2.13). From this fundamental equation all the finite-size scaling formulae in §2.3.1 can be obtained.

The standard review article for finite-size scaling is Barber (1983) which include references to the original papers in the field.

§2.3.1 The Finite-Size Scaling Formulae.

The fundamental prediction of finite-size scaling is that a physical quantity \( \Omega \) which in the bulk limit, near the critical point behaves as

\[
\Omega(t) \sim t^p ; \quad t \to 0 ,
\]

(2.14)

where \( t= (T-T_c) / T_c \) is the reduced temperature will have a finite lattice form of

\[
\Omega(M, t^*) \sim M^{p/v} Q_\Omega(t^* M^{1/v}) ,
\]

(2.15)

where \( M \) is the number of lattice sites and \( t^*=(T-T^*(M))/T^*(M) \). The pseudo critical temperature \( T^*(M) \) is the temperature where the peaks in the finite lattice specific heat occur (see Barber 1983). Equation (2.15) enables the critical exponent \( p \) to be extracted from the finite system, even though \( \Omega(M, t^*) \) itself is analytic. Specifically \( p \) is obtained from the scaling behaviour of \( \Omega(M,0) \):
\( \Omega(M, t^*=0) \sim M^{\rho/\nu} Q_\Omega(0) \)  \hspace{1cm} (2.16)

Obviously to do this we need to have already determined \( T^*(M) \) and \( \nu \).

The pseudo critical point \( T^*(M) \) can be determined as described below (following Hamer and Barber 1981a,b). When (2.16) is applied to the case where \( \Omega(M, t^*) \) is the correlation length \( \xi(M, t^*) \) we have (since \( \xi(t) \sim t^{-\nu} \) as \( t \to 0 \))

\[ \xi(M, t^*=0) \sim M \]  \hspace{1cm} (2.17)

(The assertion (2.17) can be used as the starting assumption in a heuristic derivation of (2.15) if it is further assumed that all divergent quantities \( \Omega(t) \) scale as powers of the correlation length.)

Since we will be working in the Hamiltonian formulism the equivalences listed in §1.2 can be applied to obtain the scaling behaviour of the finite-lattice mass gaps

\[ F(M, g^*=0) \sim \xi^{-1}(M, t^*=0) \sim 1/M, \]  \hspace{1cm} (2.18)

where \( g^*(g-g^*(M))/g^*(M) \). Defining the ‘scaled mass gap ratio’ \( R(M, g) \) by

\[ R(M, g) = \frac{M F(M, g)}{(M-1) F(M-1, g)} \]  \hspace{1cm} (2.19)

where the quantities on the right-hand side are numerically determined, we see using (2.18) that the pseudo critical points \( g^*(M) \) can be obtained from

\[ R(M, g^*(M)) = 1 \]  \hspace{1cm} (2.20)

The bulk critical point \( g_c \) can be found from the extrapolation of the sequence \( \{g^*(M); M=1,2, \ldots \} \).

Returning to (2.16) we recall that to determine the unknown index \( \rho \) we still need \( \nu \). The standard approach taken for determining \( \nu \) (Hamer
and Barber 1981a) is via the Callan-Symanzik beta function $\beta(g)$. In lattice gauge theory language this is defined as

$$\beta(g) = a \left( \frac{\partial g}{\partial a} \right)_{F_{\text{phys}} = \text{Const}}$$

(2.21)

where $F_{\text{phys}}$ is the mass gap in physical units. In terms of $F(g)$, $\beta(g)$ can be written (Hamer et al 1979)

$$\frac{\beta(g)}{g} = \frac{F(g)}{F(g) + g \frac{\partial F}{\partial g}}.$$  

(2.22)

For standard second order phase transitions the mass gap has the form

$$F(g) \sim \zeta^{-1}(T) \sim (g - g_c)^\nu; \quad g \to g_c.$$  

(2.23)

so the critical behaviour of $\beta(g)$ from (2.22) is

$$\beta(g) = \frac{1}{\nu} (g - g_c); \quad g \to g_c.$$  

(2.24)

Using (2.16) with $\Omega = \beta(g)$ we obtain the scaling behaviour

$$\beta(M,g) \sim M^{-1/\nu}.$$  

(2.25)

So the index $\nu$ can be found from the scaling behaviour of $\beta(M,g)$, and having obtained the pseudo critical points from (2.20), equation (2.16) can be used to find any unknown exponent $\rho$.

While (2.23)-(2.25) apply for standard phase transitions, similar results can be obtained for non-standard transitions such as the Kosterlitz-Thouless transition in the $O(2)$ model (see chapter 4 and Hamer and Barber 1981b).

Before concluding this subsection we still need a way of calculating the finite-lattice estimates of the beta function $\beta(M,g)$. There are two

\begin{footnote}
A note on nomenclature: The Callan-Symanzik function is denoted $\beta(g)$, $\beta_B = (k_B T)^{-1}$ is the Boltzmann factor, and $\beta$ is the magnetization's critical exponent.
\end{footnote}
estimates available, the first is obtained from (2.22) by replacing the bulk mass gaps on the right side by their finite lattice values (Hamer and Barber 1981a,b). A second estimate has been derived by Roomany and Wyld (1980) using an argument based on a phenomenological renormalization group. They studied a continuous finite system with periodic boundary conditions of fixed length L. Finite-lattice quantities Ω(M,T) in this scheme sample the continuous system with a spatial resolution of \( L/M \). Using this approach Roomany and Wyld obtained a finite-lattice approximate for the beta function

\[
\beta_{RW}(M,g) = \frac{\ln R(M,g)}{\ln \left( \frac{M}{M-1} \right) \left[ 1 + \frac{1}{2} g \frac{\partial}{\partial g} \ln [MF(M,g)(M-1)F(M-1,g)] \right]}
\]

This expression will be used later to form numerical estimates of the Callan-Symanzik beta function.

§2.3.2 A Renormalization Group Approach to Finite-Size Scaling

This subsection describes a derivation of the finite-size scaling law (2.15) beginning with the transformation law for correlation functions (2.13). This presentation up to the definition of the homogenous form of the singular part of the free energy density is similar to that of Barber (1977, §3.3). It should be noted that the following approach is non-standard; for the canonical and original derivation I refer the reader to §IIIA of Barber's review on the subject (Barber 1983).

The derivation begins with the transformation of the two-point correlation function under \( R_b \) which, from (2.13) is
The scale invariance principle is contained in \( (2.27) \) because the transformation \( \mathcal{R}_b \) used to derive it is merely a sophisticated scale transformation. Using translation and rotation invariance \( (2.27) \) fixes the form of the critical two-point correlation function to be

\[
\langle s(r_1) s(r_2) \rangle_{\mathcal{L}} = \frac{1}{|r_1 - r_2|^{2x}} \tag{2.28}
\]

Comparing this with the standard form \( \langle s(r_1) s(r_2) \rangle \sim |r_1 - r_2|^{-(d-2+\eta)} \) gives

\[2x = d - 2 + \eta . \tag{2.29}\]

We can define the susceptibility to be

\[\chi(t,h) = \frac{1}{M^d} \sum_{r_1, r_2} \langle s(r_1) s(r_2) \rangle_{\mathcal{L},(t,h)} \tag{2.30}\]

Using \( (2.28) \) we can find how \( \chi \) responds to the transformation \( \mathcal{R}_b \).

\[\chi(t,h) = b^{2x} \chi(b^{1/2} t, b^{1/2} h) \tag{2.31}\]

where we have also used \( (2.11) \).

The standard definition of \( \chi \) in terms of the singular part of the free energy density \( f^S \) is

\[\chi(t,h) = \frac{\partial^2}{\partial h^2} f^S(t,h) \tag{2.32}\]

This can be used to integrate \( (2.31) \) to obtain

\[f^S(t,h) = b^{2-\eta-2\eta h} f^S(b^{1/2} t, b^{1/2} h), \tag{2.33}\]

where we have used \( (2.29) \). Equation \( (2.33) \) is only valid in the
neighbourhood of the critical point where all the relevant scaling fields are
infinitesimal (see Barber 1977).

Suppose instead of a bulk system we study a finite system with $M$
sites along a linear dimension. As discussed at the beginning of §2.3 such
a system cannot be critical, so we can imagine $1/M$ as being a relevant
scaling field in the sense that the critical point is only reached as $1/M \to 0$
(see Nightingale 1982). Since under $R_{b} \frac{1}{M} \to \frac{1}{M} = b (\frac{1}{M})$ we have

$$y_{1/M} = 1.$$ \hspace{1cm} (2.34)

Renormalization group arguments can be used to also identify (see
Barber 1977)

$$y_{E} = 1/v ,$$ \hspace{1cm} (2.35)

$$y_{h} = 1/2 (d-\eta) + 1 .$$ \hspace{1cm} (2.36)

(Equation (2.36) is in fact identical to (2.29) since $y_{h} = d-x_{h} = d-x$.) Using
(2.34) and (2.36) the finite system form of (2.33) can be written

$$f^{S}(t,h,1/M) = b^{-d} f^{S}(b^{-d} t, b^{-y_{h}} h, b^{-1/M})$$ \hspace{1cm} (2.37)

Thus $f^{S}$ is a generalized homogeneous function which we have seen is a
consequence of the scale invariance principle and the covariant form of the
multi-point correlation functions (2.13). In a finite system $b=M/M'$ so
using (2.37) we can restrict the functional form of $f^{S}$ to be

$$f^{S}(t,h,1/M) = M^{-d} Y(tM^{y_{E}}, hM^{y_{h}})$$ \hspace{1cm} (2.38)

for $t,h, \frac{1}{M} \to 0$, where $Y$ is a universal scaling function (that is it is
identical for all systems within a given universality class).

Privman and Fisher (1984) have argued that (2.38) can be written as
$f^S(t,h,1/M) = M^d Y_{pp} (C_1 t^\nu Y^E, C_2 h^\nu Y^h) \text{ where } C_1 \text{ and } C_2 \text{ are the only non-universal constants appearing.}$

Finally we want to derive the fundamental finite-size scaling equation (2.15) from (2.38). This is readily achieved since every thermodynamic function can be derived in principle from the free energy. For example the singular part of the zero field specific heat $C$ is defined

$$C(M,t) = \frac{\partial^2}{\partial t^2} f^S(t,0,1/M). \quad (2.39)$$

Using (2.38), (2.35) and the scaling law $2 - \alpha = dv$ we get

$$C(M,t) = M^{\alpha/v} Q_c(t,M^{1/v}), \quad (2.40)$$

for some function $Q_c$. This is the fundamental finite-size scaling equation (2.15) applied to the specific heat. (The parameter $t^*$ in (2.15) can be replaced by $t$, see Barber 1983.)

§2.4 Conformal Invariance

This section summarizes the recent developments of conformal invariance theory. For a more detailed approach I refer the reader to the review article by Cardy (1987a). The original papers will be referenced at the appropriate points.

As discussed in §2.1, the theory of conformal invariance is based on the principle that a system at criticality is invariant when its coordinates are conformally transformed. A conformal transformation may involve local translations, rotations and dilatations (ie. the transformation of the coordinates is itself a function of position). Conformal transformations involve no shearing, so they preserve angles.
Conformal transformations are useful in other areas of physics, for example they can be applied in electrostatics since Maxwell's equations are conformally invariant.

Conformal invariance was first applied to critical field theories by Polyakov (1970). He showed that it placed constraints on the functional form of multi-point correlation functions in systems of any dimension. In particular it fixes, up to a normalizing factor, the explicit form of the three-point correlation function. We recall that scale invariance fixes the form of the two-point correlation function (see (2.28)). A simple geometric argument can be used to understand these constraints: There always exists a conformal transformation which maps three arbitrary points to three reference points, whereas a scale transformation can map at most two arbitrary points to two reference points.

The next development specific to statistical systems/field theories was made by Belavin, Polyakov and Zamolodchikov (1984a,b) hereafter referred to as BPZ. In these major works they showed that for a two dimensional critical system there is a representation of the Virasoro algebra (Virasoro 1969) corresponding to each renormalization group scaling operator. (The two-dimensional conformal group and its associated Virasoro algebra had been studied by string theorists in the 1970's in relation to the dual string model.) Furthermore, for 'minimal theories' all multi-point correlation functions of these scaling operators can be calculated in principle (since they satisfy differential equations), and all the possible scaling dimensions are known. They showed the simplest such theory corresponds to the Ising model.
Friedan, Qui and Shenker (1984), hereafter referred to as FQS showed that unitarity allowed only a discrete set of universal classes which can be labelled by an integer \( m \), where \( m = 3,4, \ldots \) They found specific models associated with the classes \( m = 3,4,5 \) and 6. The work of BPZ and FQS in outlined in §2.4.1.

Further developments were made by Huse (1984) who was able to identify models with every \( m > 6 \) and by Dotsenko and Fateev (1984) who found soluble models corresponding to each universality class and hence obtained an integral form for their multi-point correlation functions.

In a separate development, Cardy used a conformal transformation to map infinite systems to finite counterparts. This enables the (bulk) critical exponents to be extracted from finite-lattice quantities. A summary of this approach is given in §2.4.2.

§2.4.1 Two-Dimensional Infinite Systems.

This subsection follows the work of BPZ and FQS. Reference was also made to Cardy's review (1987a) and Quispel (1988).

In the rest of this section on conformal invariance attention will be restricted to two dimensions, where the powerful equivalence between conformal transformations and analytic functions on the complex plane can be used.

We begin by making the assumption that the multi-point correlation function transformation law (2.13) which has been derived for \textit{global} scale transformations also applies to \textit{local} scale transformations ie. conformal transformations. Using the renormalization group framework, this step
can be shown to be valid so long as there are only short range interactions. Since we can approximate the conformal transformation \( w(z) \) by

\[
w(z) = z_0 + w'(z_0) (z - z_0) ; \quad z = z_0
\]  

(2.41)

the scale factor at \( z_0 \) is

\[
b(z_0) = |w'(z_0)|. \quad (2.42)
\]

If we consider correlation functions involving operators \( \phi_i \) with non-zero spin dimension \( s_i \) then we can generalize (2.13) and get

\[
\langle \prod_i \Phi_i(z_i, \bar{z}_i) \rangle = \prod_i |w'(z_i)|^{\Delta_i} |w'(\bar{z}_i)|^{\bar{\Delta}_i} \langle \prod_i \Phi_i(w(z_i), \bar{w}(\bar{z}_i)) \rangle, \quad (2.43)
\]

where

\[
x_i = \Delta_i + \bar{\Delta}_i, \quad (2.44a)
\]

\[
s_i = \Delta_i - \bar{\Delta}_i, \quad (2.44b)
\]

the \( \Delta_i \) and \( \bar{\Delta}_i \) are to be determined, the bars denotes complex conjugation, and the arguments \( \bar{z}_i \) are included by convention.

Now we consider an infinitesimal transformation defined

\[
w(z) = z + \alpha_1(z) ; \quad z \in R_1
\]  

(2.45a)

\[
= z + \alpha_2(z) ; \quad z \in R_2 \subseteq \mathbb{C} - R_1. \quad (2.45b)
\]

\( R_1 \) is chosen to contain all the \( z_i \). The infinitesimal functions \( \alpha_1 \) and \( \alpha_2 \) are defined so that \( w(z) \) is analytic in \( R_1 \) and differentiable across the boundary \( \mathcal{C} \) of \( R_1 \). (Note that by Liouville’s theorem a single, non-constant, global function \( W(z), z \in \mathbb{C} \), cannot be conformal/analytic everywhere and still be infinitesimal.)

In the domain \( R_2 \) the change \( \delta \mathcal{H} \) in the Hamiltonian due to the non-conformal transformation (2.45b) can be defined in terms of the stress
tensor $T_{\mu\nu}$

$$\delta\mathcal{H} = \frac{-1}{2\pi} \int_{R_2} d^2 x \, \partial^\mu \alpha_2^\nu T_{\mu\nu}$$  \hspace{1cm} (2.46)

Since a change in the Hamiltonian will affect the microscopic states' probability distribution, the correlation functions will also change. To first order in $\alpha$ this may be written as

$$\delta \left< \prod_i \Phi_i(z_i, \bar{z}_i) \right> = \left< \delta\mathcal{H} \prod_i \Phi_i(z_i, \bar{z}_i) \right>$$  \hspace{1cm} (2.47)

In the conformal part of the domain, $R_1$, (2.43) can be used to obtain, again to first order in $\alpha$

$$\delta \left< \prod_i \Phi_i(z_i, \bar{z}_i) \right> = \sum_i \left\{ \alpha'_1(z_i) \Delta_i + \alpha_1(z_i) \frac{\partial}{\partial z_i} \right\} \left< \prod_i \Phi_i(z_i, \bar{z}_i) \right>$$  \hspace{1cm} (2.48)

Equating the two changes in the correlation function (2.47) and (2.48), we get the conformal Ward identity. Using Gauss' theorem the following local form of the conformal Ward identity is obtained

$$\left< T(z) \prod_i \Phi_i(z_i, \bar{z}_i) \right> = \sum_i \left\{ \frac{\Delta_i}{(z-z_i)^2} + \frac{1}{z-z_i} \frac{\partial}{\partial z_i} \right\} \left< \prod_i \Phi_i(z_i, \bar{z}_i) \right>$$  \hspace{1cm} (2.49)

where $z \in R_2$ and the stress tensor $T_{\mu\nu}$ has been written in terms of the coordinates $z$ and $\bar{z}$ with the component $T_{zz}(z, \bar{z})$ written as $T(z)$. (There is a similar equation to (2.49) for the component $T_{\bar{z}\bar{z}}(z, \bar{z})$.)

We now decompose the stress tensor component $T(z)$ into a Laurent series.
\[ T(z) \Phi(z_1) = \sum_{n=-\infty}^{\infty} (z - z_1)^{-2-n} L_n \Phi(z_1). \]  

\( L_n \) generates infinitesimal conformal transformations \( z \rightarrow z + \varepsilon z^{n+1} \).

Equations (2.49) and (2.50) form the basis from which all infinite geometry, two-dimensional conformal invariance results are derived.

Carrying on the BPZ approach the commutator \([T(z),T(z')]\) is derived from which \([L_n,L_m]\) can be obtained. Firstly (2.49) is used to calculate an expansion for \(\langle T(z)T(z') \rangle\) in terms of powers of \((z-z')\). The lowest order term can be written as \(c / (2(z - z')^4)\) where \(c\), the 'conformal anomaly' is a system dependent, positive constant which is not determined from (2.49).

Using cylindrical geometry and treating the \( L_n \) as quantum mechanical operators the commutator \([T(z),T(z')]\) can be found from this expansion and together with (2.50) we obtain

\[ [L_m,L_n] = (m - n) L_{m+n} + c m (m^2 - 1)/12. \]  

This is the Virasoro algebra.

The next step is to study the operators \( L_n \). We continue to interpret the \( \phi_i \) as quantum mechanical operators and the ensemble averages in (2.49) are treated as vacuum expectation values. Using (2.50) we can match the analyticity properties of both sides of (2.49) (by expanding the right side in powers of \((z-z_1)\)) and get

\[ L_n \phi_i = 0 ; \quad n > 0 \]  

and \( L_0 \phi_i = \Delta_i \phi_i \). 

The operators \( L_n, \ n > 0 \ (n < 0) \), are referred to as the lowering (raising) operators of \( L_0 \).
By analyzing correlation functions of the form \( \langle T(z_1) T(z_2) \ldots \phi(z, \bar{z}) \rangle \) and using (2.49) and (2.50) we can obtain a 'conformal block' of operators of the form

\[
\Phi_i^{(k)} = L_{-k_1} L_{-k_2} \ldots L_{-k_n} \Phi_i
\] (2.54)

where \( k_j > 0 \) and \( \{k\} = \{-k_1, -k_2, \ldots, -k_n\} \). \( \phi_i^{(k)} \) is said to be at the Nth level in the conformal block where

\[
N = \sum k_i \,,
\] (2.55)

and \( \phi_i^{(k)} \) scales, in the renormalization group sense as \( \Delta_i + N \). The operators at the zeroth level are termed 'primary' and those at all other levels are termed 'secondary'. The \( L_n, n > 0 \) (\( n < 0 \)), lower (raise) the scaling dimension of the operator it acts on by \( n \). Each conformal block \( \{\phi_i\} \) is thus closed under the generators of conformal transformations, and so is a representation of the conformal group.

We now turn to the work of FQS to complete the discussion on conformal invariance in infinite two-dimensional systems. For unitary theories, where the Hamiltonian is hermitian, all states \( \phi_i^{(k)} \| 0 \rangle \) must have non-negative norm

\[
\langle 0 | (\Phi_i^{(k)^\dagger} (\Phi_i^{(k)} \| 0 \rangle \geq 0
\] (2.56)

where \( \| 0 \rangle \) is the vacuum state. From (2.54) this norm involves products of operators \( L_{-k} \) and \( L_{-k} \). We have \( L_{-k} = L_{k} \) since the stress tensor is hermitian. The inner product (2.56) in principle can be determined using (2.51) to commute the lowering operators through the product and applying the annihilation equation (2.52). At level \( N \) the inner product defines a matrix of dimension \( P(N) \times P(N) \), where \( P(N) \) is the number of ways of partitioning the integer \( N \) (recall (2.55)). Kac (1979) has given a
form for the determinant of this matrix involving the conformal anomaly $c$ and scaling dimension $\Delta_i$ which FQS have used in their analysis. They showed the unitarity restriction (2.56) implies that possible solutions are a subset of those with zero Kac determinant and that either

$$c \geq 1$$ \hspace{1cm} \text{(2.57)}

**or**

$$c = 1 - \frac{6}{m(m + 1)} ; \quad m = 3, 4, \ldots$$ \hspace{1cm} \text{(2.58)}

and

$$\Delta_i = \frac{[(m + 1)p - mq]^2 - 1}{4m(m + 1)}$$ \hspace{1cm} \text{(2.59)}

where $p = 1, 2, \ldots, m-1$ and $q = 1, 2, \ldots, p$. (There is a similar equation for $\Delta_i$.) The conformal anomaly $c$ thus labels the universality classes. It has been shown (Cardy 1986) that if there are only a finite number of primary operators then $c < 1$. Of particular interest to this work is that Cardy (1987b) has shown that $c = 1$ corresponds to all known theories with continuously varying exponents such as the (1+1)D O(2) system.

Further information can be drawn out of the unitarity constraint. Because it implies that the determinant of the Kac matrix is zero we know that some linear combination of the raising operators $L_n$ annihilates the state $|\phi_i \rangle |0 \rangle$. The level, $N_{\text{degenerate}}$, where this occurs can be shown by the Kac formula to be $pq$ where the $p$ and $q$ define the scaling dimension of $\phi_i$ (see (2.59)). The $L_n$ can be written as differential operators (from (2.49) by expanding the right side in powers of $(z - z_i)$ and using the definition (2.50) for $L_n$) so one can write a differential equation of order $N_{\text{degenerate}}$ for correlation functions involving $\phi_i$.

It is worth summarizing the work presented in this subsection. We began assuming conformal invariance applied at the critical point so we

\footnote{which was later proved by Feigen and Fuchs (1982).}
had the conformal form of the correlation transformation equation (2.43) from which we derived the conformal Ward identity (2.49). The Laurent components $L_n$ of the stress tensor $T_{\mu\nu}$ were then found to obey the Virasoro algebra (2.51). The constraint of unitarity implied that the universality classes can be numerated and for each class the allowed scaling dimensions are known.

§2.4.2 Two-Dimensional Finite Systems.

The analysis in §2.4.1 was applied to the infinite geometry where the function $w(z)$ maps the complex plane onto itself. We are free to choose a $w(z)$ where this is not the case. Of special interest is the conformal transformation

$$z \rightarrow w(z) = \frac{M}{2\pi} \ln z$$  \hspace{1cm} (2.60)

which maps the complex plane to a finite width strip of infinite length (see figure 2.2).

---

Figure 2.2 The conformal transformation $w(z) = M/2\pi \ln z$.  

---
Several workers (Cardy 1984, Blöte et al 1986) have used this conformal transformation to relate some of the bulk properties of systems (the conformal anomaly c, and critical exponents) to some of the finite-system quantities (the correlation length along the strip and finite-size corrections to the free energy). This subsection discusses some of their results. In preparing this section reference has been made to Cardy (1987a) and Hamer (1988).

We begin by noting the form of the infinite-system two-point correlation function (cf (2.28))

$$\langle \phi(z_1) \phi(z_2) \rangle_\infty \sim |z_1 - z_2|^{-2x}. \quad (2.61)$$

Turning to the two-point form of the correlation function transformation law (2.43) - using (2.61) in the left side and the definition of w(z) (2.60) we can obtain the correlation function in the w-plane

$$\langle \Phi(u_1, v_1) \Phi(u_2, v_2) \rangle_{\text{strip}} = \frac{\left(\frac{2\pi}{M}\right)^{2x}}{[2\cosh \frac{2\pi}{M}(u_1 - u_2) - 2\cosh \frac{2\pi}{M}(v_1 - v_2)]^x} \quad (2.62)$$

where \( w(z) = u_i + v_i = w_i \). Two pieces of information will be extracted from (2.62).

(i) As \( u_1 - u_2 \to \infty \)

$$\langle \Phi(w_1) \Phi(w_2) \rangle \sim \exp\left(\frac{u_1 - u_2}{\xi(M)}\right) \quad (2.63)$$

where

$$\xi(M) = \frac{M}{2\pi x} \quad (2.64)$$

is the correlation length along the strip. This result was derived by Cardy (1984). Using the correspondences developed in §1.2 between Hamiltonian
field theory and Euclidean statistical mechanics we have the important result

\[ \text{Finite-size Mass Gap} = F(M) \sim \frac{1}{\xi(M)} = \frac{2\pi x}{M}, \]  

(2.65)

which, as with all conformal invariance results, holds at the (bulk) critical point.

(ii) A standard transfer matrix definition of the correlation function can be used to write the left side of (2.62) as a power series in \( \exp[-\pi/M(u_1 - u_2)] \). The right side of (2.62) can also be expanded in terms of the same quantity. Equating these series we get

\[ \omega_{N}(M) = \omega_0(M) + \frac{2\pi}{M} (x + N) \]  

(2.66)

where the \( \omega_{N}(M) \) are the (degenerate) finite-lattice energy eigenvalues of the system's Hamiltonian, \( \omega_0 \) is the vacuum energy and \( N \), the level of the state, is a positive integer. The eigenstate with energy \( \omega_{N}(M) \) resides in the sector corresponding with the operator whose scaling dimension is the \( x \) appearing in (2.66). This tower of states with energy spaced at \( \frac{2\pi}{M} \) corresponds exactly with the conformal block of operators \( \phi_i^{[k]} \) (see (2.54)) acting on the vacuum state \( |0> \). (See figure 2.3.)

In concluding this discussion of (2.62) we note that if we look at the level \( N = 1 \) state in (2.66) we recover (2.65).

Blöte, Cardy and Nightingale (1986) and Affleck (1986) have obtained another connection between finite-lattice and infinite-lattice quantities. Using a non-conformal transformation of the strip to define a stress tensor

\footnote{The relation (2.65) had been found empirically by several authors (Luck 1982, Derrida and de Seze 1982, Nightingale and Blöte 1983, Privaman and Fisher 1984) before it was established by Cardy (1984) to be a result of conformal invariance.}
Figure 2.3 The Energy spectrum of a strip system, also showing the correspondence with the conformal block structure of the infinite geometry.

\[ T_{\mu \nu} \] they obtained the following for the ground state energy/free energy

\[ \frac{\omega_0(M)}{M} = \omega_\infty - \frac{\pi c}{6M^2} \]  \hspace{1cm} (2.67)

where \( \omega_\infty \) is the bulk vacuum energy density and \( c \) is the conformal anomaly.

There is a complication when applying (2.65), (2.66) and (2.67) to (1+1) dimensional (Hamiltonian) field theories. While we can assume conformal invariance holds for two dimensional statistical mechanics systems, conformal invariance, specifically rotational invariance may be destroyed by the extreme anisotropic rescaling of the coordinates needed to obtain the Hamiltonian field theory (Fradkin and Susskind 1978). If rotational invariance is destroyed, it may be recovered by simply rescaling the dimension across the width of the strip. The rescaling factor \( \zeta \) is defined from the dispersion relation for fundamental excitations
where \( \omega \) and \( p \) are the energy and momentum of the lowest excited states, and \( \zeta = 1 \) for rotationally invariant systems. With this rescaling (2.65), (2.66) and (2.67) become

\[
F(M) = \frac{2\pi x \zeta}{M} \quad (2.69)
\]

\[
\omega_N(M) = \omega_0 + \frac{2\pi \zeta}{M} (x + N) \quad (2.70)
\]

and

\[
\frac{\omega_0(M)}{M} = e^{\omega_0} - \frac{\pi c \zeta}{6M^2} \quad (2.71)
\]

In most cases the dispersion relation is not known analytically so (2.68) cannot be used to determine \( \zeta \). In these cases some numerical juggling has to be done to determine the desired bulk quantities \( x \) and \( c \) from (2.69) - (2.71). This will be done in §4.3.3 for the (1+1)D O(2) model and the exponent \( \eta (= 2x_h, \text{see (2.29)}) \), the scaling dimension \( x_E \) and the conformal anomaly \( c \) are found.

In summarizing this chapter we have seen that the finite-size scaling equations (see §2.3.1) are a means of determining the critical point and the exponents from finite-lattice quantities. Conformal invariance (see §2.4) completes the armoury available to extrapolate to the bulk behaviour. Specifically it can be used to determine the conformal anomaly (universality class) of the system and the scaling dimensions/critical exponents from critical ‘amplitudes’ measured on the finite-lattice. Both finite-size scaling and conformal invariance have been shown to be ‘derivable’ from a renormalization group formulation. Finally these comments beg the question: How are the finite-lattice solutions determined? This question will be answered in the next chapter.
Chapter 3
Truncation Schemes and Eigensolution Methods

"Scepticism can combine with the egalitarian dislike of cleverness to oversimplify even the simplest issues and also to an increasing distrust of the expert."
- Donald Horne.

§3.1 Introduction

In chapter 2 the finite-size scaling and conformal invariance equations were derived which enable the bulk properties of the system of interest to be extracted from the finite-lattice solutions. This represents the second half of the Hamiltonian finite-lattice approach. The first half, that of obtaining the finite-lattice solutions from the model's Hamiltonian, will be outlined in this chapter. The ubiquitous harmonic oscillator will be placed on a discrete lattice and used as a test-bed for the various methods of solving the Hamiltonian of a finite system.

The problem of finding the lowest energy eigensolutions of a Hamiltonian appears in many branches of physics and there is a correspondingly large number of algorithms available. Attention will be restricted to the various eigensolution methods that have been applied to finite-lattice Hamiltonian field theories.

The ultimate aim in all of these approaches is to use the eigensolutions obtained in the finite-size scaling and conformal invariance
equations ((2.16)-(2.26) and (2.69)-(2.71)) to extract the critical point, the
critical indices and, for two dimensional systems, the conformal anomaly.
Data from each lattice size (or pair of lattice sizes) are used in these
equations to give an estimate of the bulk quantity of interest. To obtain the
most accurate final result (i) accurate finite-lattice data and (ii) data from
a large number of lattice sizes are required. In general these two
requirements are difficult to satisfy due to the huge dimensions of the state
space in even the simplest models on small lattices. This is particularly
exemplified in cases where either (i) the finite-lattice Hilbert space is
infinite dimensional (eg. the O(2) model where each site has an infinite
number of states) or (ii) the number of spatial dimensions is two or more
so that although the finite-lattice Hilbert space may be finite, its
dimensions grow so rapidly with lattice size that only the smallest few
lattices are computationally manageable. Thus the two requirements
imply that eligible Hamiltonian eigensolution methods should *efficiently
truncate* the basis while *maintaining accuracy*. It is against this criteria
that the various methods are judged.

There are two halves to the Hamiltonian solution algorithms. They
are shown schematically in figure 3.1. The first part is given a
Hamiltonian and a choice of basis, use a truncation scheme to generate
(numerically or sometimes analytically) the Hamiltonian matrix
elements. The second part is computing the lowest eigensolutions from
the Hamiltonian matrix obtained in part 1. Some truncation schemes are
iterative in the sense that at each order the truncated Hamiltonian matrix
is adjusted as a function of the eigenvector obtained at the previous order.
In these iterative schemes the above two-stage procedure is repeated until convergence in the eigenvalue is obtained.

![Diagram](image)

Figure 3.1 A representation of the stages involved in solving the lowest states of a finite-lattice Hamiltonian problem.

In §3.2 choices of basis sets and various truncation schemes are reviewed and a selection of the truncation schemes are applied to the test-bed model: the lattice harmonic oscillator (LHO). Section 3.3 briefly outlines some of the many numerical algorithms available to calculate the eigensolutions of a given matrix. The methods used in the case of the O(2) and Z(2) models (in chapters 4 and 5) are discussed in both sections.

§3.2 Truncation Schemes and the Lattice Harmonic Oscillator.

This section discusses the choices of bases to represent the Hamiltonian and studies five truncation schemes, four of which are
applied to the LHO. These four are deterministic in nature, and two of these schemes will be applied to the (1+1)D O(2) model in chapter 4. The fifth scheme, 'stochastic truncation', uses a Monte-Carlo approach to restrict the number of basis states and is tested on the (2+1)D Z(2) model in chapter 5.

The problem at hand is to generate a matrix representation for Hamiltonians of the form

$$H = H_0 - xV$$

(3.1)

where $x$ plays the role of a coupling parameter or inverse temperature (see Kogut 1979).

The immediate task is to choose a basis to represent the Hamiltonian. There are two obvious choices. Most commonly a basis set is chosen which diagonalizes $H$ in the strong coupling limit ($x = 0$). This has been used by a number of workers in the field for example Hamer and Barber (1981a,b) and Roomany et al (1980). The second choice is the basis which diagonalizes the weak coupling limit ($x \to \infty$) of the Hamiltonian $H$. This has been used in variational approaches to the problem (Choe et al 1988) which have been discussed in §1.3. Since the weak coupling basis was not applied in these projects it will not be discussed any further.

To set notation, the strong coupling basis states will be denoted by $|I\rangle$ and their (unperturbed) energies $\langle I|H_0|I\rangle$ by $E(I)$. The eigenstates of $H$ are denoted $||i\rangle$ and they have energy eigenvalues of $\omega_I = \langle i|H|i\rangle$. Note states $|I\rangle$ and $||i\rangle$ are normalized to one. This notation is used throughout the dissertation.

The strong coupling basis states are generated by successive applications of the perturbation operator to some initial state $|0\rangle$ (Hamer
et al 1979). Usually $|0\rangle$ is chosen to be the strong coupling ground state $|0\rangle_{x=0}$. The 'order' of the state $|I\rangle$ is equal to the number of times the operator $V$ has to be applied to $|0\rangle$ to first form the state $|I\rangle$. Since periodic boundary conditions are enforced throughout these projects the states $|I\rangle$ are defined so that they are translationally invariant. In the case of the LHO, the basis states $|I\rangle$ and matrix elements $\langle I|H|J\rangle$ can be determined analytically. However it is more usual for this to become cumbersome and a numerical algorithm (such as that outlined in chapter 4) to be used.

As already outlined in §3.1, the major problem with the strong coupling basis is the incredibly large number of basis states needed to span the eigenvectors in the weak coupling regime accurately. This is a serious problem because it is this $x \rightarrow \infty$ limit which is the physically interesting region since it represents the continuum limit for asymptotically free theories. This problem is illustrated in table 3.1 where the number of strong coupling basis states that significantly contribute to the ground state $|0\rangle$ of the 4-site $(1+1)D \ O(2)$ model is listed at various couplings $x$. ('Contribute significantly' is defined here to mean that the amplitude of state $|I\rangle$ in the ground state $|0\rangle$ exceeds $10^{-5}$. ie. $\langle I|0\rangle > 10^{-5}$.)

Having laid the groundwork on the choice and generation of the basis, and reinforced the need for an 'efficient, accurate' basis set truncation scheme, attention will now be focussed on the LHO.

The LHO was first used as a testing ground for lattice gauge theories by Jurkiewicz and Wosiek (1978) where it was solved exactly and used to test the Padé method of finding the weak coupling limit. Hamer (1979) used the LHO in the first application of finite-lattice techniques to
Hamiltonian field theories. The harmonic oscillator on a lattice is a useful practice model for lattice gauge theorists since it displays some of the analytic features and singularities of lattice field theories and it is exactly soluble both on the lattice and in the continuum.

<table>
<thead>
<tr>
<th>x</th>
<th>Number of strong coupling states</th>
<th>11 &gt; with &lt;11 &gt; &gt; 10^{-5}</th>
</tr>
</thead>
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<td>1.</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>53</td>
<td></td>
</tr>
<tr>
<td>5.</td>
<td>92</td>
<td></td>
</tr>
<tr>
<td>10.</td>
<td>139</td>
<td></td>
</tr>
<tr>
<td>20.</td>
<td>214</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.1 Number of states needed to accurately span ground state of the 4-site (1+1)D O(2) model as x increases.

The continuum Hamiltonian for the harmonic oscillator is

$$H_0^{\text{continuum}} = -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{1}{2} k z^2.$$  (3.2)

It has the familiar harmonic oscillator energy eigenvalues

$$\omega_i^{\text{continuum}} = (i + \frac{1}{2}) \sqrt{\frac{k}{m}} ; \quad i = 0, 1, ...$$  (3.3)

Following Hamer and replacing the continuum z coordinate with a lattice labelled by odd integers

$$z = n a ; \quad n = \pm 1, \pm 3, ...$$  (3.4)

the lattice Hamiltonian becomes

$$H^{\text{lattice}} = \frac{1}{2} k a^2 [\hat{n}^2 + x (2 - \hat{d}_- - \hat{d}_+) ]$$  (3.5)
where the operators $\hat{n}$ and $\hat{d}_{\pm}$ act on the position eigenstates $|n\rangle$:

\[
\hat{n} |n\rangle = n |n\rangle, \\
\hat{d}_{\pm} |n\rangle = |n \pm 2\rangle
\]

and the lattice coupling parameter $x$ is defined

\[
x = \frac{1}{4 m k a^4}.
\]

Note that $x$ is inversely proportional to the continuum coupling $k$ and that $x \to \infty$ corresponds to the continuum limit $a \to 0$. These features are typical for a lattice coupling constant.

For convenience a reduced Hamiltonian $H$ is defined:

\[
H = \frac{2}{ka^2} H^{\text{lattice}} = H_0 + x V.
\]

This is in the standard form (3.1) with

\[
H_0 = \hat{n}^2
\]

and $V = 2 - \hat{d}_+ - \hat{d}_-.

For our purposes only the even-parity position states need be discussed. Following the earlier description on the generation of the strong coupling basis we define the even parity, translationally invariant zeroth state to be

\[
|0\rangle = \frac{1}{\sqrt{2}} [ |1\rangle + |-1\rangle].
\]

All other strong coupling basis states $|I\rangle$ are generated by successive applications of $V$ to $|0\rangle$.

In the strong coupling representation the Hamiltonian matrix elements $H_{IJ}$ ($I,J = 0,1,\ldots$) are easily found to be

\[
H_{0,0} = 1 + x \\
H_{IJ} = (2I+1)^2 + 2x; \quad I > 0
\]
The tridiagonal nature of the LHO Hamiltonian is not a feature shared by spin systems of lattice gauge models.

The lowest eigenvalue of $H$ is a characteristic value of the Mathieu equation (Jurkiewicz and Wosiek 1978)

$$\omega_0(x) = 1 + x - \frac{1}{8} x^2 + \ldots$$

(3.14)

which has a continuum limit $x \to \infty$ of

$$\omega_0(x) \to 2 \sqrt{x}; \quad x \to \infty$$

(3.15)

and, when rescaled to the units of $H^{\text{lattice}}$ (see (3.9)), corresponds to the continuum value of $\omega_0^{\text{continuum}}$ as in (3.3).

The aim of the rest of this section is to test four truncation schemes to see which one most accurately and efficiently gives the continuum limit (3.15) in the weak coupling region. The truncation schemes are:

I Naive Truncation (Outer projection)

This scheme defines a subspace $S$ of the full strong coupling basis and only states $|I\rangle \in S$ are considered in the calculation. The eigen-equation for this scheme is

$$H^I \|i\rangle^I = \omega^I_1 \|i\rangle^I$$

(3.16)

where

$$H^I = O^I (H_0 + V) O^I$$

(3.17)

is the truncated Hamiltonian, $\omega^I_1$ and $\|i\rangle^I$ are the eigensolutions obtained from this scheme, and $O^I$ is the projection operator onto $S$. The eigenvalues $\omega^I_1$ for this scheme are upper bounds to the true eigenvalues
\( \omega \) (Löwdin 1965). The naive truncation scheme effectively sets the amplitudes in the eigenvectors of those states outside the subspace to zero.

Obviously the subspace \( S \) should reflect the physics of the problem so that basis states which contribute significantly to the full eigenvector \( |i\rangle \) will be included in \( S \). For spin models or lattice gauge models there are several natural choices of \( S \) available (Irving and Hamer 1983). For example \( S \) may be defined to include only basis states \( |I\rangle \) whose unperturbed energies \( E(I) \) are less than some cut-off \( E_{\text{max}} \). Various definitions of \( S \) are tested in chapter 4 on the O(2) model.

For the LHO the choice of \( S \) is restricted by the simplicity of the model to the 'order-N cut-off':

\[
S = \{ |I\rangle : \text{order of } |I\rangle \leq N \}. \tag{3.18}
\]

Thus the strong coupling representation of \( H^I \) is (using (3.13))

\[
H_{IJ}^I = H_{IJ}; \quad I,J = 0,1,\ldots,N. \tag{3.19}
\]

The effect of the naive cut-off (and the other truncation schemes) on an idealized wavefunction is shown schematically in figure 3.2.

II Healing Algorithm - Continuous Derivative

The healing algorithm takes some account of the states outside the subspace \( S \) that are ignored in the naive truncation scheme. Specifically it includes, in an approximate manner, the contribution to the eigenstate \( |i\rangle \) of states \( |I'\rangle \) which are outside \( S \) but are connected to the states \( |I\rangle \) inside the subspace via the perturbation operator \( V \) (ie. \( \langle I' | V | I \rangle \neq 0 \)). The effect of the states \( |I'\rangle \) is included in the algorithm by obtaining an approximate value of \( \langle I'|i\rangle \) in terms of the amplitudes \( \langle I|i\rangle \) and by
adjusting the matrix elements of the naively truncated Hamiltonian accordingly, as described below.

In scheme II the amplitude \( \langle I' \| i \rangle \) is approximated by assuming that the 'derivative' of the amplitude is continuous across the 'boundary' of the subspace \( S \). For the LHO where \( S \) is defined via the order \( N \) cut-off and the state referred to above as \( \ket{I'} \) is the \((N+1)\)th order basis state \( \ket{N+1} \) the condition for 'continuous derivative' is

\[
\langle N+1 \| i \rangle - \langle N \| i \rangle = \langle N \| i \rangle - \langle N-1 \| i \rangle
\]

Some simple algebra shows that with this definition of \( \langle N+1 \| i \rangle \) the scheme II Hamiltonian \( H^\Pi \) can be defined in terms of the naively truncated Hamiltonian matrix \( H^I_{I,J} \) \((I,J = 0,1, \ldots, N)\) by

\[
H^\Pi_{N,N-1} = 0
\]

\[
H^\Pi_{N,N} = H^I_{N,N} - 2x
\]

\[
H^\Pi_{I,J} = H^I_{I,J} \quad \text{otherwise}
\]

\[\text{Figure 3.2 Representation of the eigenfunctions obtained in the different truncation schemes.}\]
III Healing Algorithm - Exponential Fit

This section follows the same ideas of scheme II except in the way the amplitude(s) \( \langle I' \| i \rangle \) are approximated. This method has been applied to the ground state eigensolution where empirically the amplitudes fall off as an exponential of the unperturbed energy of the corresponding basis state. Thus \( \langle I' \| 0 \rangle \) is approximated by

\[
\langle I' \| 0 \rangle \approx \exp\{-c_1 E(I')\}
\]

for some constant \( c_1 \). An iterative approach is used in this scheme. The first step in the process is to obtain an eigenvector and to fit the amplitudes to the exponential form \( \langle I \| 0 \rangle \approx \exp\{-c_1 E(I)\} \) to obtain \( c_1 \). Then (3.22) is used to approximate \( \langle I' \| 0 \rangle \) which in turn is used to define the matrix elements \( H_{ij}^{III} \). For the LHO these are

\[
H_{NN}^{III} = H_{NN}^I - x \exp\{-c_1(2N+1)\} \quad (3.23a)
\]
\[
H_{LJ}^{III} = H_{LJ}^I \quad \text{otherwise.} \quad (3.23b)
\]

The eigenequation \( H^{III} \| 0 \rangle^{III} = \omega_0^{III} \| 0 \rangle^{III} \) is solved and the process is iterated until \( \omega_0^{III} \) converges.

IV Inner Projection.

This method was introduced to solve the time-independent Schrödinger equation by Bazley and Fox (1961). It gives a lower bound to the true eigenvalues of \( H \). The method in its simplest form involves the inversion of the matrix \( \langle p_i | V | p_j \rangle \) where \( | p_i \rangle \) \( (i = 0, 1, ... \) are linearly independent states, in our case they'll be the strong coupling basis states \( | I \rangle \). The Hamiltonian is re-written as

\[
H^{IV} = H_0 - x VP^K
\]

where \( VP^K \) is defined by
\[ \mathbf{V} \mathbf{P}^K = \sum_{i,j=0}^{K} \mathbf{V} | p_i \rangle b_{ij} \langle p_j | \mathbf{V} \]  

with \( b_{ij} \) the elements of the inverse of \( \langle p_k | \mathbf{V} | p_i \rangle \), \((i,j,k,l = 0,1, \ldots K)\).

\( \mathbf{V} \mathbf{P}^K \) has the property that

\[ 0 \leq \langle \varphi | \mathbf{V} \mathbf{P}^K | \varphi \rangle \leq \langle \varphi | \mathbf{V}^K+1 | \varphi \rangle \leq \langle \varphi | \mathbf{V} | \varphi \rangle \]  

for any \( | \varphi \rangle \), so the eigenvalues \( \omega_1^{IV} \) satisfy \( \omega_1^{IV} \leq \omega_1^{IV} \leq \omega_1 \).

In cases where the matrix representation \( \langle p_i | \mathbf{V} | p_j \rangle \) is tridiagonal, such as the LHO (3.25) can be simplified and \( \langle p_i | \mathbf{V} \mathbf{P}^K | p_j \rangle \) can be written as a tridiagonal matrix of dimension \( K+2 \). For the LHO \( H^{IV} \) is defined:

\[ H^{IV}_{N,N} = H^{I}_{N,N} - x \]  

\[ H^{IV}_{L,J} = H_{L,J} \quad \text{otherwise} \]

where \( | p_i \rangle = | I \rangle \). Here \( K \) has been chosen to equal \( N-1 \) so that the dimension of \( \mathbf{V} \mathbf{P}^K \) is the same as the other truncated Hamiltonians.

The four truncation schemes are applied to the LHO at a number of cut-offs \( N \). The eigensolutions of the matrices were computed using standard numerical packages. (For more complicated models the matrices involved are huge and the methods of §3.3 have to be used to compute the eigensolutions.) The two lowest even-parity (rescaled) eigenvalues \( \omega_0(x)/\sqrt{x} \) and \( \omega_2(x)/\sqrt{x} \) for the four truncation schemes are plotted versus \( 1/\sqrt{x} \) in figures 3.3 (\( N = 2 \)) and 3.4 (\( N = 5 \)), together with the bulk lattice result.

Recalling that the aim of the exercise is to obtain information on the continuum limit \( 1/\sqrt{x} = 2\sqrt{(mk)} a^2 \rightarrow 0 \), see (3.3), (3.8) and (3.15)), it is clear that schemes II and IV (continuous derivative and inner projection) are least accurate and that scheme III (exponential fit) is most accurate.
Figure 3.3 Plots of the two lowest even-parity (rescaled) eigenvalues a) $\omega_0(x)/\sqrt{x}$ and b) $\omega_2(x)/\sqrt{x}$ against $1/\sqrt{x}$ for the harmonic oscillator. The results for each of the 4 truncation schemes are shown. This figure calculates the eigenvalues using the cut-off at $N = 2$.

Figure 3.4 As in figure 3.3 except the cut-off used is $N = 5$. 
(Schemes I and IV provide upper and lower bounds as predicted.) However as well as accuracy, the criteria for choosing the best truncation algorithm includes efficiency and it is here that scheme III (exponential fit) falls down. It is the only iterative scheme and the number of iterations (each involving the diagonalization of the Hamiltonian matrix) required for six figure accuracy ranges between 2 and 50. At a given cut-off N, the scheme requires more iterations for convergence the closer the coupling is to the weak coupling limit.

In conclusion, based on these tests, scheme I (naive truncation) is probably the most successful truncation algorithm, but scheme III (exponential fit), depending on the number of iterations required, is worth further testing on more complicated models. As a result of these findings both schemes are applied to the (1+1)D O(2) model in chapter 4.

To complete this section on truncation schemes a fifth algorithm, ‘stochastic truncation’, is discussed. This is not applied to the LHO because its statistical nature makes it difficult to directly compare with the other (deterministic) truncation schemes. It is discussed here because it is applied to the (2+1)D Z(2) model in chapter 5.

V Stochastic Truncation

This novel scheme (Hamer 1987) relies on a non-deterministic approach to truncating the basis space. A full explanation of the algorithm will appear later (chapter 5).

Stochastic truncation involves a number of statistical estimates of the ground state’s eigenvalue and eigenvector at successive iteration steps. It is based on the power method (§3.3) except that the trial ground state
vector's components are 'statistically integerized' after each application of the (full) Hamiltonian. Some of the components whose amplitudes lie between 0 and 1 will be zeroed, 'truncating' the corresponding state from the basis. The statistical integerization is carried out in a manner which keeps the number of non-zero components roughly constant throughout the iteration.

§3.3 Matrix Eigensolution Algorithms.

This section describes the numerical procedures that were used in chapters 4 and 5 to evaluate the lowest eigensolutions of the finite lattice Hamiltonians (see figure 3.1). It also indicates why these methods were chosen from the vast array of matrix eigensolution packages available.

Throughout this section certain characteristics of the matrices generated by the methods of §3.2 will need to be kept in mind. In general the matrices will be (i) large (with dimensions up to hundreds of thousands), (ii) sparse (number of non-zero elements of the order of 10-20 times the matrix dimension), and (iii) real and symmetric. In addition it should be emphasized that only the lowest two eigenvalues and their corresponding eigenvectors need be found for the successful extraction of the bulk critical behaviour of the system (part two of the finite-lattice Hamiltonian approach - see chapter 2).

The large number of algorithms available for determining the eigensolutions of matrices can be classified (Bradbury and Fletcher 1966) into two types (I) transformation methods (eg. the Householder procedure) and (II) iterative methods. The first algorithm type won't be considered since they are inefficient for large, sparse matrices due to 'fill-in'
problems. There are several common routines that fall into the iterative category:

(i) those involving the Rayleigh quotient $\frac{\langle \varphi | H | \varphi \rangle}{\langle \varphi | \varphi \rangle}$ eg. method of steepest descent, conjugate gradient, and the Davidon procedure (see Bradbury and Fletcher for a discussion and references). The most efficient of these methods for our class of problems is the conjugate gradient method, but this still doesn't converge as quickly (at least in certain circumstances, see Hamer 1983) as the Lanczos scheme (see later). Curiously though it has recently been shown (Burkitt and Irving 1988) that both the conjugate gradient and Lanczos methods, when used for finding inverses, are different parameterizations of the same scheme. However since the Rayleigh quotient methods were not applied to any models, they will not be discussed any further.

(ii) the power method. This method is based on the approximation

$$\text{largest eigenvalue of } A = \frac{\langle \psi^0 | A^N | \psi^0 \rangle}{\langle \psi^0 | A^{N-1} | \psi^0 \rangle} \quad \text{as } N \to \infty \quad (3.28)$$

for any starting vector $| \psi^0 \rangle$ with non-zero overlap with the eigenvector of $A$ corresponding to the largest eigenvalue. For Hamiltonian theories, to find the lowest energy states the matrix $A$ is defined

$$A = E_{\text{max}} - H \quad (3.29)$$

for some appropriate value of the constant $E_{\text{max}}$. The stochastic truncation scheme (scheme V, §3.2) is a statistical algorithm based on (3.28). Since the power method itself is not as efficient as the Lanczos scheme it will not be discussed further, and the stochastic truncation scheme will be described fully in chapter 5.
(iii) the Lanczos class of algorithms (Lanczos 1950). These have a long history of application to physical problems, being particularly useful to nuclear physicists working with shell model calculations (Whitehead et al 1977). The Lanczos procedure was first applied to Hamiltonian lattice theories by Hamer and Barber (1980, 1981a,b) and Roomany et al (1980).

The rest of this section is devoted to the Lanczos scheme and its generalizations. The original algorithm will be described firstly, followed by the variant on it which was used in chapter 4 on the O(2) model. The section concludes with comments on some of the other Lanczos based procedures that have been applied to Hamiltonian lattice theories.

The Lanczos scheme generates an orthonormal basis $|\varphi^n\rangle$ and a matrix representation on this basis which is tridiagonal for hermitian matrices. The steps can be summarized as follows.

(i) Begin with a 'Lanczos starting vector' $|\varphi^0\rangle$. For our models this was chosen to be

$$|\varphi^0\rangle = c_0 \sum_{I=0}^{M} \exp\{-c_1 E(I)\} |I\rangle$$

(3.30)

where $c_0$ and $c_1$ are constants chosen so that $\langle \varphi^0 | \varphi^0 \rangle = 1$. This form for $|\varphi^0\rangle$ reflects the empirical behaviour of the lowest eigenstates.

(ii) Multiply with $\hat{H}$ to generate a new Lanczos vector $|\varphi^1\rangle$,

$$\hat{H} |\varphi^0\rangle = a_0 |\varphi^0\rangle + b_1 |\varphi^1\rangle$$

(3.31)

or in general,
\[ \mathbf{H} |\varphi^n\rangle = b_n |\varphi^{n-1}\rangle + a_n |\varphi^n\rangle + b_{n+1} |\varphi^{n+1}\rangle. \]  
(3.32)

The state \( |\varphi^{n+1}\rangle \) is defined so that \( (\varphi^m |\varphi^n\rangle = \delta_{m,n} \). (This matrix multiplication in our case is carried out in the strong coupling basis.)

(iii) Calculate \( a_0 \) and \( b_1 \) from (3.31), or in general \( a_n \) and \( b_{n+1} \) from (3.32) to get the tridiagonal matrix representation:

\[
\mathbf{H}^{nth-Lanczos'} = \begin{bmatrix}
  a_0 & b_1 & 0 \\
  b_1 & a_1 & b_2 \\
  & & \ddots & \ddots \\
  & & & b_n \\
  0 & & & b_n & a_n
\end{bmatrix}
\]  
(3.33)

(iv) Go to step (ii).

One of the advantages of the Lanczos scheme is that the eigenvalues \( \omega_i^{nth-Lanczos'} \) converge (Whitehead et al 1977) to the true eigenvalues \( \omega_i \) as \( n \) increases, with the fastest convergence being in the eigenvalues at the extremes of the spectrum.

The above describes the standard Lanczos scheme. The 'N-step' or 'nested' Lanczos procedure used in chapter 4 is a simple variant of the above algorithm. It is a generalization of the 2-step method of Berger et al (1977) and involves the additional step:

(v) After \( N \) of the above iterations, find the lowest eigenvalue, \( \omega_0^{Nth-Lanczos} \) and corresponding eigenvector, \( |0\rangle^{Nth-Lanczos} \) of \( \mathbf{H}^{Nth-Lanczos} \) let \( |\varphi^0\rangle = |0\rangle^{Nth-Lanczos} \) and repeat the above procedure from step (i). The eigensolutions \( \omega_0^{Nth-Lanczos} \) and \( |0\rangle^{Nth-Lanczos} \) converge to the true eigensolutions \( \omega_i \) and \( |0\rangle \) as the number of outside iterations increase.
The advantages in this N-step procedure compared with the original Lanczos scheme is its saving in storage. In the N-step procedure only N+1 ‘Lanczos vectors’ $|\varphi^n\rangle$ and a small $(N+1)\times(N+1)$ tridiagonal matrix need to be stored. (Note each $|\varphi^n\rangle$ is stored in its strong coupling basis form.)

The value of N actually used is a compromise between fast convergence (N large) and small storage requirements (N small). The value $N = 10$ was chosen. (Note $N = 1$ corresponds to the power method.)

The lowest excited state of the Hamiltonian can be found in the N-step Lanczos procedure by firstly converging onto the ground state, and then setting the starting Lanczos vector $|\varphi^0\rangle$ to the second lowest eigenvector of $H^{N_{th-Lanczos}}$. To obtain correct convergence onto the excited state, each Lanczos vector $|\varphi^n\rangle$ is orthogonalized with respect to the ground state.

Note that the matrix multiplication in step (ii) is easiest to carry out using the strong coupling basis, so the matrix $H$ should firstly be represented on this basis.

The last remarks in this section will be directed towards some other variants of the Lanczos scheme outlined in Alberty et al (1984) and Patkós and Ruján (1985). Both of these papers propose methods to control the explosion in the number of strong coupling basis states necessary to map out the eigenstates as the lattice coupling $x$ increases.

The first paper introduces two concurrently running schemes to iteratively approach the eigensolution. The first scheme, ‘coupling subdivision’ solves (subject to the second scheme) the Hamiltonian at coupling $x_n = n/N \times x$ where $n$ is the iteration number, $N$ the total number of iterations and $x$ the coupling where the solution is actually required. The second scheme, ‘subspace extension’ is based on the 2-step Lanczos
procedure, however at the n\textsuperscript{th} iteration a solution to the problem at coupling \( x_n \) is found \textit{within a restricted subspace} \( S_n \) rather than the full space (see Alberty et al for details). Once the eigenvector at coupling \( x_n \) is found within \( S_n \) it is used as the starting vector at the \( (n+1) \text{th} \) iteration. The subspaces \( S_n \) should fill out to accurately span the full eigenvector at coupling \( x_n = x \).

This method gives good convergence, but its main advantage, a small storage requirement only holds in the early iterations since at the final coupling \( x_N = x \), the subspace \( S_N \) must still be large enough to accurately span the full eigenvector. The time saving feature of diagonalizing a small (2x2) matrix is also apparent in the N-step Lanczos routine described above. The idea of Alberty et al of coupling subdivision is to some extent utilized in the O(2) and Z(2) projects. Usually the eigensolutions are required for several couplings \{\( x_j \)\}, so the eigenvector at \( x_i \) can be 'handed-down' as the starting Lanczos vector for the calculation at coupling \( x_{i+1} \).

The second paper (Patkós and Ruján 1985) tests a 'basis vector importance sampler' (BVIS) and a variational starting vector for the Lanczos procedure. They also incorporate a BVIS to the methods of Alberty et al. The BVIS throws away strong coupling basis states whose overlaps with the trial eigenvector is less than a certain cut-off. The dimension needed to determine the ground state energy to six decimal places in this scheme for O(2) chains can be reduced by a factor of 2 to 4 from standard 'fixed-subspace' methods (Patkos and Rujan). However a similar result can be achieved by a simpler scheme - that of the naive
truncation scheme where the cut-off plays the role of the BVIS (see chapter 4).

While the use of a variationally optimized starting vector for the Lanczos scheme provides a more accurate eigenvalue estimate early in the iteration sequence, unfortunately a useful level of convergence requires around the same number of Lanczos iterations as the unoptimized start (Patkos and Rujan). In any case for the O(2) model, the starting vector was chosen to have an exponential decay in the unperturbed energy which although isn’t variationally optimized roughly maps the form of the actual eigenvector.

In summarizing this chapter, it has been argued that the (deterministic) method of basis space truncation which is likely to provide the best compromise between efficiency and accuracy is the naive truncation scheme with a physically relevant subspace. It has also been shown that an exponential model of the healing algorithm warrants further investigation. The conclusion regarding eigensolution packages for our problem types (finding the lowest couple of eigenvalues and their eigenvectors of large, sparse matrices) is that the N-step Lanczos procedure appears to best compromise storage, accuracy and speed. This algorithm can be improved by choosing a starting Lanczos vector close to the shape of the true eigenvector and by a ‘hand-me-down’ of eigenvectors when a solution at more than one coupling is desired.

Chapters 2 and 3 have laid the foundations for the finite-lattice Hamiltonian study of spin systems/gauge theories by describing the mathematical rules and computational algorithmns to be followed. These
are now applied to the two major projects of this dissertation. For the O(2) chain, (chapter 4) a combination of naive truncation and the N-step Lanczos algorithm described above are used for the eigensolving, and finite-size scaling and conformal invariance are used to analyse the finite-lattice data. In the second project, (chapter 5) the stochastic truncation algorithm itself is tested by applying it to the (2+1)D Z(2) model. Finite-size scaling is used to see what accuracy can be gained from the method.
Chapter 4

The (1+1)D O(2) Model

"The time has come," the Walrus said,
"To talk of many things,
Of shoes - and ships - and sealing wax -
Of cabbages and kings -
Of why the sea is boiling hot -
And whether pigs have wings ..."

- Lewis Carroll,
Alice in Wonderland.

§4.1 Introduction

§4.1.1 The Model

This chapter presents an analysis of the two-dimensional O(2) or planar rotator model whose partition function is defined as

\[ Z = \prod_{\text{sites } i} \int d\phi_i \exp\left(-\frac{J}{k_B T} \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j)\right), \tag{4.1} \]

where the sites \( i \) and \( j \) lie on a two-dimensional lattice, \( \phi_i \in [0,2\pi) \) is the direction of the spin at site \( i \) measured relative to an arbitrary axis, \( J \) is the coupling and the sum is over nearest neighbour sites \( i \) and \( j \).

This model has been intensely studied because of its unusual phase structure but has defied an exact solution. It has been proved (Mermin and Wagner 1966) that it must have zero spontaneous magnetization for non-zero temperatures and yet there has long been evidence of a phase transition (see eg. Stanley 1968).
This apparent contradiction was resolved by Kosterlitz and Thouless (1973) who proposed a new definition of long-range order based on the topological properties of the system. Although the system has zero long-range order in the conventional sense (and hence zero spontaneous magnetization), the presence of topological order does indicate a 'topological' phase transition.

Kosterlitz and Thouless hypothesized that the mechanism responsible for the transition is the unbinding of vortex-antivortex pairs. At low temperatures they showed that 'spin waves' dominate the system causing the two-point correlation function to vanish algebraically with separation. In this phase the vortices are tightly bound together in pairs and hence there is topological order. As the temperature increases these vortex pairs unbind, disordering the system, causing correlations to vanish exponentially with separation.

Thus the model has a standard high temperature phase above some temperature $T_c$ and a low temperature region made up of a line of critical points (since the correlation function vanishes algebraically in this region).

The different forms of the correlation function in the two regions imply that the correlation length must have a singularity. From a renormalization analysis Kosterlitz (1974) obtained the following functional form for the correlation length:

$$\xi \sim \exp \left[ b \left( \frac{T_c}{T - T_c} \right)^\sigma \right]; \quad T > T_c, \quad (4.2a)$$

$$= \infty \quad ; \quad T \leq T_c, \quad (4.2b)$$

where $\sigma = 1/2$. 
The model is believed to have no singularity in its specific heat (Hamer and Barber 1981b) so the corresponding critical exponent $\alpha$ is identically zero. This means (through the scaling relations between the exponents) that there is only one critical exponent to be determined which we will take to be the correlation function exponent $\eta$ (ie. with $\alpha = 0$ all critical exponents can be written in terms of $\eta$). Unlike second order transitions, the exponent $\eta$ can be defined throughout the low-temperature region, and is found to vary with coupling.

Aside from its interesting statistical mechanics behaviour, the $O(2)$ model is of interest to quantum field theorists as it has the same renormalization group structure as the 4-dimensional $U(1)$ gauge theory ie. quantum electrodynamics (Migdal 1975). The model also describes the critical behaviour of a thin film of atomic oxygen on a tungsten substrate and the superfluid phase transition in thin films of He$^4$ (Kosterlitz and Thouless 1973, Bishop and Reppy 1978, Dash 1978).

This chapter continues with a summary of the methods used to date in the study of the model and a description of the approach taken in this analysis. Section 4.2 details the finite-lattice Hamiltonian method (cf §§3.2 and 3.3) and §4.3 outlines the extraction of the bulk critical quantities from the finite-lattice results (cf. §2.3 and §2.4).

§4.1.2 Summary of the Methods Used to Study the 2D O(2) Model.

Since 1973 there have been many attempts to accurately pin down the position of the phase transition $T_c$ and the critical parameters $\eta$ and $\sigma$. A list of some of these methods are outlined in table 4.1 which categorizes them according to figure 1.2 and briefly describes their methods. Because
Table 4.1 A list of some of the analyses of the 2-dimensional O(2) model (cf. Fig 1.2 for classifications).

\[ \tau_c = k_B T_c/J, \quad \eta \text{ is the correlation function index at } \tau_c, \quad \sigma \text{ is defined in (4.2), and the coupling } \chi \text{ is defined in (4.4).} \]  
The critical points shown in square brackets refer to the Luther and Scalapino model, and cannot be directly compared with the canonical O(2) model.

<table>
<thead>
<tr>
<th>Authors Details of Method</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical Point</td>
<td>[ \eta, \sigma ]</td>
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<table>
<thead>
<tr>
<th>Authors</th>
<th>Details of Method</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferer and Velgakis 1983</td>
<td>12th order high temperature series</td>
<td>[ T_c=1.45\pm0.02, \eta=27\pm0.03, \sigma=5.1\pm1 ]</td>
</tr>
<tr>
<td>Luck 1982</td>
<td>low temperature series</td>
<td>[ T_c=9 ]</td>
</tr>
<tr>
<td>Hamer et al 1979</td>
<td>strong coupling series for mass gap</td>
<td>[ x_c=1.7 ]</td>
</tr>
<tr>
<td>Hornby and Barber 1985</td>
<td>ditto</td>
<td>[ x_c=1.78\pm0.04, \eta=50\pm0.08 ]</td>
</tr>
<tr>
<td>Hamer and Kogut 1979</td>
<td>strong coupling series for susceptibility</td>
<td>[ x_c=1.8\pm1, \eta=7\pm1 ]</td>
</tr>
<tr>
<td>Guttmann et al 1988</td>
<td>ditto</td>
<td>[ x_c=1.86\pm0.06 ]</td>
</tr>
<tr>
<td>Hamber and Richardson 1981</td>
<td>str coupl on Luther&amp;Scalapino model</td>
<td>[ [x_c=3.4], \eta=27\pm1, \sigma=85\pm4 ]</td>
</tr>
</tbody>
</table>

**REnormalization Group**

| Kosterlitz 1974 | includes interaction between vortices | \[ T_c=1.35, \eta=1/4, \sigma=1/2 \] |
| Migdal 1975 | block recursion relation | \[ \tau_c=1.0 \] |
| Droz and Malaspinas 1978 | real space decimation | \[ \tau_c=1.026, \eta=\sigma=1/2 \] |

**VARIATIONAL**

| Heys and Stump 1987 | 2-parameter trial wavefunction | \[ \eta=1.35, \sigma=1/4 \] |
| Kosterlitz and Thouless 1973 | considered vortex unbinding | \[ \tau_c=1.35, \eta=1/4 \] |
| Stump 1980 | spin 1/2 approximation | \[ \tau_c=1.0 \] |
| Mattis 1984,1985 | approximate map onto XXZ model | \[ \tau_c=0.883, \eta=1/2 \] |
| Luther and Scalapino 1977 | truncated spins to 0 & \pm1 | \[ [\tau_c=4/\pi], \eta=1/4 \] |
| den Nijs 1982 | corrected above for 'umklapp' process | \[ \tau_c=1.026, \eta=1/4 \] |
| Nienhuis 1982 | critical hexagonal O(n) maps to 6 vertex | \[ \tau_c=1.9, \eta=1/4 \] |
| Baxter 1986 | solves loop model \rightarrow crit. hex. O(n) sol'n | \[ \tau_c=1.9, \eta=1/4 \] |
| Batchelor and Blöte 1988 | used above for finite lattice solution | \[ \tau_c=1.9, \eta=1/4 \] |

**NUMERICAL:**

**MONTE CARLO**

| Tobochnik and Chester 1979 | (Euclidean) Metropolis up to \( 100^2 \) | \[ \tau_c=0.89, \eta=0.25, \sigma=0.7 \] |
| Fernández et al 1986 | ditto up to \( 200^2 \) | \[ \tau_c=0.89, \eta=0.24, \sigma=0.03 \] |
| Van Himbergen 1984 | ditto up to \( 50^2 \) using helicity | \[ \tau_c=0.793, \eta=0.24 \] |
| Heys and Stump 1984 | (Hamiltonian) Greens functionMC | \[ \tau_c=0.9 \] |

**EXACT FINITE-LATTICE**

| Roomany and Wyld 1980 | finite-lattice sol'n using str coupl basis | \[ \tau_c=1.9, \eta=0.51, \sigma=0.01 \] |
| Hamer and Barber 1981b | ditto | \[ \tau_c=1.8, \eta=0.9 \] |
| Barber and Richardson 1981 | finite-lattice study of Luther&Scal. | \[ \tau_c=2, \eta=0.25 \] |
| Kolb et al 1982 | ditto | \[ \tau_c=2.2 \] |

**USING O(2) AS A TEST-BED FOR NUMERICAL METHODS**

| Stump 1985 | projector (Euclidean) Monte Carlo | \[ \tau_c=0.89 \] |
| Kogut and Polonyi 1986 | comparing microcanonical and Metropolis | \[ \tau_c=0.89 \] |
| Askew et al 1986 | testing performance of transputers | \[ \tau_c=0.89 \] |
| Dagotto and Kogut 1987 | accelerated and hybrid molecular dynamics | \[ \tau_c=0.89 \] |
of its subtle phase structure it has been used by several workers as a test-
bed model for numerical algorithms. Some of these projects are listed at
the end of the table. As can be seen from table 4.1 there exists large varia-
tions in the estimates of the critical point and the exponents $\eta$ and $\sigma$.

A few of the papers listed in table 4.1 will be commented on below. Those whose critical point predictions are in square brackets are for the
Luther and Scalapino approximation to the full O(2) model. This method
treats a simpler model which has only three states per site, but still re-
tains the O(2) global symmetry. It is identical to a 'naive' spin truncation
scheme to be discussed in §4.2.2. From universality arguments the criti-
cal indices will be identical to that of the canonical O(2) model (4.1), but the
critical points of the two models are not expected to be related.

Another important sequence of papers is that of Nienhuis (1982), Bax-
ter (1986) and Batchelor and Blöte (1988). They deal with a model with O(n)
symmetry whose partition function is

$$Z = \prod_{\text{sites } k} \left\{ \int d\vec{s}_k \right\} \prod_{\langle ij \rangle} \left[ 1 + \lambda \vec{s}_i \cdot \vec{s}_j \right] \tag{4.3}$$

where the second product is over nearest-neighbours $i$ and $j$ on a hexago-
nal lattice and the $\vec{s}_i$ are n-component spins.

Nienhuis was able to derive a mapping of this model for $-2 \leq n \leq 2$, via
the 'loop' model, onto a parameterization of the six-vertex model. He also
showed that an antiferromagnetic Potts model on a triangular lattice is
equivalent to the same six-vertex model if the parameters of the O(n) and
Potts models take special values. Using the known behaviour of the six-
vertex model under renormalization group transformations, he argued
that the original O(n) model must be critical when it takes these special va-
values of its parameters. (Nienhuis’s parameter constraints for (4.3) can be thought of as applying along a line in the \((n,x)\) space.)

Baxter was able to solve Nienhuis’s loop model and hence the critical \(O(n)\) model. Batchelor and Blöte used this bulk solution to obtain a finite-lattice solution and hence (from conformal invariance) the critical indices and conformal class of the model. For \(n = 2\) they obtained \(\eta = 2x_n = \frac{1}{4}\) and conjectured \(x_E = 2\).

Unfortunately the \(O(n)\) model (4.3) is not the canonical one (ie. for \(n=2\) it is not (4.1)) and it is also on a hexagonal rather than square-lattice, so Nienhuis’s value of the critical point is not related to the canonical square-lattice critical point. Thus despite this work, the canonical \(O(2)\) model’s critical point has not been found rigourously. In appendix A the quantum Hamiltonian corresponding to (4.3) is derived and is found to be identical with the Hamiltonian for (4.1) (ie. it is (4.4)). Unfortunately, Baxter’s solution is only for the isotropic case so \(x_c\) cannot be found from this method.

§4.1.3 Summary of the Approach Taken.

In this chapter a finite-lattice Hamiltonian approach (Hamer and Barber 1981a,b) is used to analyse the \(1+1)D O(2)\) model. The aim of the project is to determine as accurately as possible the critical parameters of the model and to determine its conformal invariance universality class (ie. conformal anomaly). It is hoped that some methods will be developed here which will be applicable to lattice gauge theories.

The next section defines the Hamiltonian appropriate for the system. Since the model has an infinite number of states per site, the finite-lattice Hamiltonian is infinite-dimensional and a basis state truncation scheme
is essential. Various truncation schemes are tested in §4.2.2, the most efficient being used for the rest of the calculation (cf. §3.2). Section 4.2.3 raises some computational issues involving algorithms and memory requirements. The standard techniques of finite-size scaling and conformal invariance (see §§2.3,2.4) are used to determine the bulk behaviour from the finite-lattice solutions in §4.3. The position of the critical point $x_c$ is determined, the index $\eta$ is found as a function of coupling, the Kosterlitz-Thouless value of $\sigma^{-1/2}$ is confirmed, and the conformal class of the system is shown to be $c = 1$.

The results of this work have been published: Allton and Hamer (1988). The following report of the analysis is similar to that paper, but in a slightly more detailed form.

§4.2 Method

§4.2.1 The O(2) Hamiltonian.

The O(2) system (4.1) can be realized as a Hamiltonian field theory on a one-dimensional lattice with a continuous time dimension (Fradkin and Susskind 1978, Hamer et al 1979). In the angular momentum representation the M-site quantum Hamiltonian is (cf. (3.1))

$$
H = \sum_{m=1}^{M} \left[ J^2(m) - \frac{x}{2} \left( J_+(m) J_-(m+1) + J_-(m) J_+(m+1) \right) \right. \\
\left. - \frac{h}{2} \left( J_+(m) + J_-(m) \right) \right] \tag{4.4a}
$$

$$
= H_0 - \frac{x}{2} V - \frac{h}{2} W \tag{4.4b}
$$

with commutators

$$
[J(m), J_\pm(m')] = \pm J_\pm(m) \delta_{m,m'} \tag{4.4c}
$$
where $J(m)$ measures the spin at each site, $J_+/(m)$ are the raising/lowering operators and $h$ is the magnetic coupling. Periodic boundary conditions are used. The thermal coupling $x$ is defined in terms of the temperature like variable (see table 1.1 and Hamer et al 1979)

$$x = \frac{2}{g^2}.$$  (4.5)

This form for the lattice coupling is typical for the Hamiltonian approach. Normally the high (low) temperature region maps onto small (large) values of the Hamiltonian lattice coupling parameter (recall (3.8) for the lattice harmonic oscillator).

The finite-lattice method used to extract the energy eigenstates of the Hamiltonian is based on the work of Hamer and Barber (1981a,b). The strong coupling basis states $|I\rangle$ and the corresponding representation of the M-site Hamiltonian are generated according to the procedure outlined in §3.2 and §4.2.3. The eigensolutions are obtained using an N-step Lanczos procedure (see §3.3).

The zero magnetic field Hamiltonian commutes with the total spin operator $S = \sum_m J(m)$, so the spectrum of eigenstates forms sectors labelled by the value of $\langle S \rangle$. There are four eigenstates of interest to us: the ground and first excited states in the $\langle S \rangle = 0$ sector (defined $|0\rangle$ and $|2\rangle$ respectively) and the ground and first excited states in the $\langle S \rangle = 1$ sector (defined $|1\rangle$ and $|3\rangle$). These states have energies $\omega_i$ ($i = 0$ to 3). The mass gap between states $|i\rangle$ and $|j\rangle$ is defined $F_{ij} = \omega_i - \omega_j$ with $F_{01} = F$.

§4.2.2 Truncation Schemes.

In the strong-coupling ($x=0$), angular momentum representation each lattice spin can take on any integer value, so clearly even the finite-
lattice Hamiltonian is infinite-dimensional. A further restriction on these strong coupling states \( |I\rangle \) is obviously necessary to make the finite-size model computationally tractable. Some possible truncation schemes have already been tested in §3.2 on the lattice harmonic oscillator and using the conclusions reached there, the 'naive truncation' (scheme I) is applied to the model and the 'healing algorithm-exponential fit' (scheme III) is tested further.

Unlike the lattice harmonic oscillator, there are several different ways of implementing the naive truncation scheme (Irving and Hamer 1983). These define the subspace \( S \) (see §3.2) by using the

(i) **Order of formation** (only strong coupling states \( |I\rangle \) formed up to the Nth order are considered - see §3.2),

(ii) **Spin** (the spins \( J(m) \) at each site \( m \) are restricted so that \( |\langle I|J(m)|I\rangle| \leq J_{\text{max}} \), and

(iii) **Unperturbed energy** (only states \( |I\rangle \) with \( E(I) = \langle I|H_0|I\rangle \leq E_{\text{max}} \) are included).

These three naive truncation methods were applied to a 6-site test lattice at \( x = 2.0 \) to find which was most efficient. It turned out that the third method (limiting the unperturbed energy) gives the most accurate eigenvalue for a given dimension of the subspace \( S \). This is displayed in Figure 4.1 where the accuracy of the ground state energy \( \omega_0 \) for all three methods is plotted against the dimension of \( S \). The value of \( x = 2.0 \) was chosen because it lies close to (if not on!) the value of the critical point \( x_c \). Note the improvement in efficiency is similar to that in the basis vector importance sampler of Patkós and Ruján discussed in §3.3, but easier to implement.
The healing algorithm using an exponential fit was also tested (scheme III, §3.2). As described in §3.2 this involved an iterative process, fitting an exponential to the eigenvector and correcting the Hamiltonian matrix for the states lying 'just' outside the subspace $S$. In this implementation of the scheme a value for $c_1$ (see (3.22)) is obtained at step (v) of the N-step Lanczos procedure (see §3.3) and the Hamiltonian is adjusted accordingly at this step (cf. (3.23)). The N-step Lanczos procedure continues as usual until convergence is obtained. Table 4.2 indicates the improve-
ment in the accuracy of the ground state eigenvalue from a test run using a six-site lattice with various values of the energy cut-off $E_{\text{max}}$.

<table>
<thead>
<tr>
<th>$E_{\text{max}}$</th>
<th>Naive Truncation (Energy cut-off)</th>
<th>Healing Algorithmn Exponential Fit</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>$1.1 \times 10^{-3}$</td>
<td>$5.4 \times 10^{-4}$</td>
</tr>
<tr>
<td>40</td>
<td>$2.8 \times 10^{-7}$</td>
<td>$1.9 \times 10^{-7}$</td>
</tr>
<tr>
<td>60</td>
<td>$2.1 \times 10^{-10}$</td>
<td>$1.3 \times 10^{-10}$</td>
</tr>
</tbody>
</table>

As can be seen from the table the improvement in accuracy is much less than an order of magnitude and is not commensurate with the computational complexity introduced in the healing algorithm scheme. Unfortunately, for this reason the healing algorithm was discarded and the energy truncation scheme retained as the cut-off scheme used in the 'production runs'.

§4.2.3 Numerical/Algorithmic Details.

This subsection overviews the computational side of the project. It details the important (ie. time consuming) sections of the computer code and shows how they can be written efficiently. The 'raw' CPU time and memory requirements are also discussed.

The first part of the computer code to be outlined here is the algorithm described in figure 3.1 by the box titled 'Apply truncation scheme to
get matrix $H'$. This part of the code generates the strong coupling basis states $|I\rangle$ 'order by order' and defines the Hamiltonian matrix $H_{ij}$ (see §3.2).

A significant reduction in the number of basis states is possible if 'symmetrized' states are used. Because periodic boundary conditions are used and the Hamiltonian (4.4) is invariant under translations, reflections and spin inversions $J(m) \rightarrow -J(m)$, $m = 1,\ldots,M$, the basis states $|I\rangle$ can be restricted to also having these symmetry invariances. These transformations will be denoted $\Omega_L$, $L = 1,\ldots,4M$.

Thus a typical basis state on a three site lattice might be

$$|I\rangle = \frac{1}{\sqrt{6}} \{ |1\rangle \otimes |0\rangle \otimes |1\rangle + |1\rangle \otimes |1\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle \otimes |1\rangle$$

$$+ |1\rangle \otimes |0\rangle \otimes |1\rangle - |1\rangle \otimes |1\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle \otimes |1\rangle \}$$

(4.6)

where the product state $|J_1\rangle \otimes |J_2\rangle \otimes |J_3\rangle$ refers to the state whose spin at site $m$ is $\langle I|J(m)|I\rangle = J_m$, $m = 1,2,3$. In general, (4.6) can be written

$$|I\rangle = \frac{1}{\sqrt{Q_1}} \sum_{i=1}^{\alpha_1} |I; i\rangle$$

(4.7)

where $|I; i\rangle$ is one of the product states $|J_1\rangle \otimes |J_2\rangle \otimes \ldots |J_M\rangle$.

The basis state $|I\rangle$ may be defined uniquely by choosing a representative state from $\{ |I; i\rangle; i = 1,\ldots,\alpha_1 \}$ which will be denoted $|I; 1\rangle$. The full (symmetrized) state $|I\rangle$ can be reconstructed if needed from the representative state $|I; 1\rangle$.

The representative state $|I; 1\rangle$ in turn is stored most efficiently as a 'spin code' in one word of memory using the following scheme

$$\text{spin code of } |I; 1\rangle = \sum_{m=1}^{M} (J_m + K)^{m-1}$$

(4.8)

by choosing the constant $K$ large enough so that each spin code corre-
sponds to a unique state. (There will be an absolute maximum value that \( |J_m| \) can take due to the energy cut-off discussed in the previous section.)

All of the above is standard in the field (see Hamer and Barber 1981b, and the appendices of Roomany et al 1980, Hamer 1983, Hamer and Johnson 1986).

A computer algorithm which generates the \((N+1)\)th order states from the \(N\)th order states using the application of the operator \( V \) (as discussed in §3.2) is presented as follows:-

(i) 'Decode' the spin code of the \(N\)th order representative state \( |I;1\>_N \) using (4.8) in reverse to get the \( J_m, \ m = 1,\ldots,M. \)

(ii) Generate the spin codes for all \(4M\) states \( \Omega_L |I;1\>_N, \ L = 1,\ldots,4M \)

For each \( m, \ m = 1,\ldots,M \)

(iii) For each \( L, \ L = 1,\ldots,4M; \) Form the spin code of the \((N+1)\)th order state \( |J;L\>_N+1 \) by 'perturbing' the spin codes of the state \( \Omega_L |I;1\>_N \) with the (local) perturbation operators \( J_{+,\kappa}(\Omega_L(m))J_{-,\kappa}(\Omega_L(m+1)) \) (see (4.4a)). (When the magnetic field \( h \) is non-zero the local perturbation operators \( J_{+,\kappa}(m) \) are also used.)

(iii) If the unperturbed energy of the newly formed state is greater than \( E_{\text{max}} \) then it is ignored.

(iii) Find the representative state \( |J;1\>_N+1 \) of the \(4M\) newly formed states.

This algorithm works with the spin codes as much as possible (rather than the values of the spins at each site) and, importantly, only has to use the time consuming (4.8) to calculate spin codes \(4M\) times (step (ii)). An earlier algorithm doesn't have step (ii) so that the perturbation is done on the individual spins \( J_m \) and the spin code calculation (4.8) has to be
carried out $4M$ times \textit{every time} a local perturbation operator is applied. The new algorithm saves a factor of two in the total time spent in steps (i) to (iii).

So far the algorithm which generates the basis states $|I\rangle$ has been discussed. The code to calculate the elements $H_{IJ}$ can easily be incorporated into the above algorithm. It is not difficult to prove that the matrix element

$$
N+1 \langle J | V | I \rangle_N = \gamma_{I \rightarrow J} \sqrt{\frac{\alpha_I}{\alpha_J}}
$$

where $\gamma_{I \rightarrow J}$ is the number of times the representative state $|J;1\rangle_{N+1}$ is obtained from a local perturbation operation acting on $|I;1\rangle_N$. However it can be proved using the symmetry property $V = V^\dagger$ that

$$
N+1 \langle J | V | I \rangle_N = \sqrt{\gamma_{I \rightarrow J} \gamma_{J \rightarrow I}} = \sqrt{\text{integer}}
$$

Since integers generally require half as much memory as reals, the storage requirements for the Hamiltonian matrix can thus be halved if the square of the element is stored in \textit{integer} format rather than storing the actual matrix element as a real number.

This completes the discussion of the algorithm for the second box in figure 3.1. The algorithm for the third box in figure 3.1 (labelled §3.3) involves the N-step Lanczos routine (§3.3). The 'core' (ie. most time intensive) routine in this algorithm is the multiplication of the Hamiltonian matrix by the Lanczos vector (see step (ii) of the Lanczos procedure, §3.3, and the appendix of Hamer and Johnson 1986). While this is straightforward to code on a scalar machine it is difficult to write an efficient code for vector machines due to the sparseness of the Hamiltonian matrix. Appendix B details a code which has overcome these difficulties.
In the N-step Lanczos routine, N was chosen to be 10 and the eigenvalue converged to one part in $10^{-12}$ within 10 of the outside loops (i.e. within the 10th loop of steps (i) to (v) in §3.3, so $H$ was applied less than 100 times).

The programme used to set up the Hamiltonian matrix and solve for the energy eigensolutions totals around 1000 lines of FORTRAN code. A DEC Vax computer was used for the 1 to 7 site calculations and a Cyber 205 supercomputer with a code optimized for vector efficiency was used to solve 8 and 9 site lattices. Table 4.3 illustrates the rapid growth in computing power and storage requirements that are involved as the lattice size increases.

The barrier to moving to still larger lattices on the Cyber 205 is memory limitations, not excessive CPU time. The total memory needed for a 9-site lattice with a basis state energy cut-off of 30 units exceeds the main memory of the machine. Page faulting becomes by far the dominant component of the nominal cost of the machine and thus limits the size of lattices that can be handled.

<table>
<thead>
<tr>
<th>M</th>
<th>Machine</th>
<th>Energy &quot;cut-off&quot;</th>
<th>Dimension of Hamiltonian</th>
<th>Number of non-zero matrix elements</th>
<th>CPU time taken forming:</th>
<th>Accuracy of eigenvalue (at $x = 2.0$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Matrix(secs)</td>
<td>One eigen-solution(secs)</td>
</tr>
<tr>
<td>7</td>
<td>VAX 780</td>
<td>60 units</td>
<td>16,026</td>
<td>106,316</td>
<td>-2000 secs</td>
<td>-700 secs</td>
</tr>
<tr>
<td>8</td>
<td>Cyber 205</td>
<td>40 units</td>
<td>23,943</td>
<td>290,000</td>
<td>-28 secs</td>
<td>-3 secs</td>
</tr>
<tr>
<td>9</td>
<td>Cyber 205</td>
<td>30 units</td>
<td>34,891</td>
<td>440,000</td>
<td>-92 secs</td>
<td>-6 secs</td>
</tr>
</tbody>
</table>
§4.3 Results

§4.3.1 Critical Point

The first point of interest in the model lies in the determination of the critical point. We use three methods to find $x_c$:

(i) using finite-size scaling to determine where the mass gap scales as $\frac{1}{M}$ (see §2.3.1);

(ii) fitting the numerically obtained Callan-Symanzik $\beta$ function to the $\beta$ function obtained from Kosterlitz's suggested form of the mass gap (ie. the inverse of (4.2)) (see Roomany and Wyld 1980);

(iii) extrapolating the finite-size mass gaps directly to the bulk limit using the Romberg algorithm (this method follows that used by Beleznay 1986).

§4.3.1.1 The Critical Point from the Scaling of the Mass Gap.

Following through §2.3.1 we can define $R(M,x)$ as in (2.19) and note that the pseudo-critical point $x_c^*(M)$ can be defined by $R(M,x_c^*(M)) = 1$ (cf. (2.20)). We can improve on this method by introducing an 'M-shift' (Hamer and Barber 1981c) by defining $R(M,x,\varepsilon)$ by

$$R(M,x,\varepsilon) = \frac{(M + \varepsilon) F(M,x)}{(M - 1 + \varepsilon) F(M-1,x)} \quad (4.11)$$

The pseudo-critical points $x_c^*(M,\varepsilon)$ are defined by $R(M,x_c^*(M,\varepsilon),\varepsilon) = 1$ and are extrapolated in $M$ to give $x_c(\varepsilon)$. The result for one particular extrapolation routine is shown in figure 4.2.
In the limit of large $M$, the $x_c(\epsilon)$ values should not depend on $\epsilon$, so the estimate of $x_c$ is given by the flat part of the curve. From figure 4.2 I estimate $x_c = 1.9\pm0.1$.

There are many different algorithms available to extrapolate the sequence $\{x_c^*(M,\epsilon); M = 1, 2, \ldots\}$. The best method found was the 'alternating VBS' algorithm (Barber and Hamer 1982, Vanden Broeck and Schwartz 1979). This is the one used in figure 4.2. Another method, that of Lubkin (1952), generally did not give such consistent results.

\begin{center}
\begin{figure}
\centering
\includegraphics[width=\textwidth]{critical_point}
\caption{Critical point $x_c$ against the extrapolation parameter $\epsilon$. These results are obtained using the alternating VBS algorithm (see §4.3.1.1). The plots are from lattice sizes $M = 1, 2, \ldots, 7$ and $M = 1, 2, \ldots, 9$ as indicated. The estimate from this curve is $x_c = 1.9\pm0.1$.}
\end{figure}
\end{center}
§4.3.1.2 The Critical Point from the Callan-Symanzik $\beta$ function.

The standard definition of the $\beta$ function in terms of the mass gap is given by (2.22). Near the critical point the $O(2)$ model's mass gap behaviour is (the inverse of ) (4.2). When this is substituted into (2.22) the following form for $\beta(g)$ is obtained:

$$\frac{\beta(g)}{g} \sim (g - g_c)^{1+\sigma}. \quad (4.12)$$

A numerical estimate of the bulk $\beta$ function is obtained from extrapolating the finite-size $\beta^{RW}(M,g)$ from (2.26) to the $M = \infty$ limit. Again there is a choice of lattice sizes to use in the extrapolation sequence and a choice of extrapolating algorithms to use. The most consistent estimate of $\beta(g)$ is from the VBS algorithm using the lattice sizes $M = 1, 2, ..., 8$. This numerically obtained $\beta$ function is fitted to Kosterlitz's parameterized form (4.12) using a three parameter least-squares fit. The best fit was

$$x_c = \frac{2}{g_c^2} = 2.06 \pm 0.04 \quad (4.13a)$$

$$\sigma = 0.501 \pm 0.005. \quad (4.13b)$$

These compare favourably with value Kosterlitz derived from his approximate solution of the model (ie. $\sigma = \frac{1}{2}$) and agree with the results obtained by Roomany and Wyld (1980) using a similar fitting procedure.

§4.3.1.3 The Critical Point from a Romberg Mass Gap Extrapolation.

This method follows that of Beleznay (1986). It employs the Romberg algorithm to extrapolate a sequence of finite-size mass gaps to the bulk limit assuming an expansion of the finite-size mass gaps in powers of $\frac{1}{M}$. Every possible combination of lattice sizes is used to form the sequence of mass gaps. (The Romberg algorithm can be applied to mass gaps from
non-sequential lattice sizes.) Those sequences that converge give $x_c=2.0$. The logarithms of the bulk mass gaps for a few sequences of lattice sizes (M=1,2,...,5; M=1,2,...,6 and M=1,2,...,7) are shown in figure 4.3. The Romberg algorithm also gives an upper bound for the error of the estimate. From this method using all the converging sequences of lattice sizes, we estimate $x_c = 2.00\pm0.03$. This confirms the results of Beleznay.

Figure 4.3 Log (base 10) of mass gaps from the Romberg extrapolation against coupling $x$, plotted here for a variety of lattice sizes as shown. This approach is described in §4.3.1.3. The mass gaps extrapolate to negative values in the region indicated. (In this region the log of the absolute value of the mass gaps is shown.) From curves such as these the estimate $x_c = 2.00\pm0.03$ was obtained.
§4.3.2 The Index $\eta$.

§4.3.2.1 A Finite-Size Scaling Estimate of $\eta$.

For standard phase transitions the mass gap approaches zero in the vicinity of the critical point as

$$F \sim (g - g_c)^\gamma.$$  \hfill (4.14)

However, since the mass gap for this model has an exponential form (see (4.2)), $\nu$ itself cannot be defined. Similarly the exponents of the magnetization $M$ and susceptibility $\chi$ ($\beta$ and $\gamma$ respectively) do not have standard definitions. However if $M$ and $\chi$ are expressed in terms of the correlation length $\xi$ one can make sensible definitions of related exponents $\tilde{\beta} = \beta/\nu$ and $\tilde{\gamma} = \gamma/\nu$ and continue to use finite-size scaling as usual (see (2.14)-(2.16)),

$$\chi_M \sim \xi^{\tilde{\gamma}} \sim M^{\tilde{\gamma}} ; \quad M \to \infty$$  \hfill (4.15a)

$$M_M \sim \xi^{\tilde{\beta}} \sim M^{\tilde{\beta}} ; \quad M \to \infty$$  \hfill (4.15b)

(see Kosterlitz 1974). The usual strong scaling laws give

$$\tilde{\gamma} = 2 - \eta$$  \hfill (4.16a)

$$\tilde{\beta} = \eta/2$$  \hfill (4.16b)

so that as expected the transition is effectively described by a single magnetic index $\eta$.

A finite-lattice estimate of the susceptibility $\chi$ can be obtained from both

$$\chi_M = \frac{1}{M^2} \sum_{i=1}^{M} \sum_{m=1}^{M} \langle 0 \mid V(i,m) \mid 0 \rangle$$  \hfill (4.17a)

where
\[ V(i,m) = J_+(i) J_+(m) + J_-(i) J_-(m) \]  

(see Pesch and Kroemer 1985) and

\[ \chi_M = \frac{\partial^2 \omega_0}{\partial h^2} \bigg|_{h=0} \]  

(4.18)

(using the equivalence with statistical mechanics). We obtain the magnetization \( M \) from (see Hamer 1982):

\[ M_M = \frac{1}{M} \sum_{m=1}^{M} \langle \langle 1 \| J_+(m) + J_-(m) \| 0 \rangle \rangle \]  

(4.19)

We see that to obtain \( \chi \) and \( M \) the lowest eigenstates must be known.

The exponent \( \eta \) can be determined from the \( \chi_M \) and \( M_M \) ((4.17)-(4.19)) via the respective finite-size scaling relations \( \chi_M \sim M^{2-\eta} \) and \( M_M \sim M^{-\eta/2} \) (using (4.15) and (4.16)). Thus each of (4.17), (4.18) and (4.19) gives an independent estimate of \( \eta \) which will be labelled \( \eta^a \), \( \eta^b \) and \( \eta^c \) respectively.

The best method for extracting the exponent from these scaling relations of the form \( \Phi_M \sim M^\alpha \) is as follows:

\[ \alpha = \lim_{M \to \infty} (M + \varepsilon) \left( \frac{\Phi_M}{\Phi_{M-1}} - 1 \right) \]  

(4.20)

The limiting process was facilitated with the VBS algorithm. Columns 2, 3 and 4 of table 4.4, and figure 4.4 show \( \eta_{a,b,c}(x) \) determined in this way. There is excellent agreement between the methods.

\section{4.3.2.2 Other Estimates of \( \eta \)}

The results for the index \( \eta \) can be compared with some analytical expectations:

(i) As \( T \to 0 \) (or \( x \to \infty \)), the low-temperature series analysis of Luck (1982) predicts for the Euclidean version of the model
\eta(T) \sim \frac{T}{2\pi} ; \quad \text{as } T \to 0 . \quad (4.21)

A weak-coupling analysis of Hamer (outlined in Appendix 2 of Allton and Hamer 1988) gives the equivalent result

\eta(x) \sim \frac{1}{\pi \sqrt{2x}} ; \quad x \to \infty . \quad (4.22)

Note that (4.21) and (4.22) match exactly if we use the equivalences $x = 2/g^2$ and $g = T$ (see (4.5) and table 1.1). This weak-coupling prediction (4.22) is listed in table 4.4 as $\eta^{wc}$ and plotted in figure 4.4. The data appear quite consistent with this asymptotic behaviour.

---

**Figure 4.4** Plots of estimates of the critical index $\eta$ against coupling $x$. The plots shown are of $\eta^{a)$ from table 4.4 (which was obtained from the susceptibility (4.17)) and the weak and strong coupling expansions (described in §4.3.2.2). The other estimates of $\eta$ in table 4.4 ($\eta^{b)}$, $\eta^{c)}$, $2x_{01}$ and $2x_{20}$) are not shown as they are within a few per cent of $\eta^{a)}$. 

---
Table 4.4 Estimates of the critical exponent $\eta$ and scaling dimensions $x_{ij}$ of the $O(2)$ model. $\eta^{a)}$, $\eta^{b)}$ and $\eta^{c)}$ are defined in §4.3.2.1 and $\eta^{wc)}$ is from the weak coupling expansion (4.22). The scaling dimensions $x_{ij}$ are determined from the method outlined in §4.3.3. The error in the data is of the order of the last figure shown. We expect $\eta = 2x_1 = 2x_{01} = 2x_{23}$ and $x_{02} = x_{13} = x_2 = 2$ in the critical region.

<table>
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<th>$x$</th>
<th>$\eta^{a)}$</th>
<th>$\eta^{b)}$</th>
<th>$\eta^{c)}$</th>
<th>$\eta^{wc)}$</th>
<th>$2x_{01}$</th>
<th>$2x_{23}$</th>
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<td>0.129</td>
<td>0.131</td>
<td>2.04</td>
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</table>
(ii) As $T \to T_c^-$, the renormalization group analysis of Kosterlitz (1974) predicts (see table 4.1)

$$\eta(T) \sim \frac{1}{4} - \alpha (T_c - T)^{1/2}; \quad T \to T_c^-$$

of in terms of the coupling $x$

$$\eta(x) \sim \frac{1}{4} - \alpha' (x - x_c)^{1/2}; \quad x \to x_c^+.$$  \hspace{1cm} (4.24)

The result $\eta(x_c) = \frac{1}{4}$ is now known to be exact (Batchelor and Blöte 1988). The predictions of $\eta(x_c)$ obtained from $\eta^{a,b,c}$ differ from this value, remaining below $\eta = \frac{1}{4}$ to within the estimated errors throughout the region $x = 1.8 \to 2.0$ where the critical point is expected to lie. This may be caused by the presence of logarithmic corrections to scaling at the critical point. Such logarithmic corrections are known to occur in the case of the XXZ Heisenberg model (Alcaraz et al 1987) which is a soluble model with a Kosterlitz-Thouless transition. They render the convergence of the finite-lattice results very slow in the vicinity of the transition point, with a corresponding decrease in accuracy of the estimated exponent.

(iii) 'High temperature' or strong coupling series data is the last analytic method to give predictions for $\eta$. Series for the mass gap were given by Hamer et al (1979) and for the susceptibility by Hamer and Kogut (1979) (see table 4.1). The series for the mass gap was subsequently extended to tenth order by Hornby and Barber (1985), and that of the susceptibility to 8th order by Guttmann et al (1988) (see also Allton and Hamer 1988).

Hamer and Kogut (1979) outlined a way of estimating the critical exponent $\eta$ using these series. They formed the quantity

$$- \frac{D \log x}{D \log F} \sim 2 - \eta; \quad g \to g_c$$

using (4.15a) and (4.16a), and estimated it using Padé approximants.
Using this relationship and the extended series, Hamer defined the quantity \( \eta \) in the high-temperature regime (Allton and Hamer 1988). The result is shown in figure 4.4. Again, this estimate of \( \eta \) does not agree with the prediction \( \eta(x_c) = \frac{1}{4} \). This is not unexpected, since the Padé approximants will not be able to mimic a singular, cusp-like behaviour such as (4.24) in the vicinity of the transition point.

§4.3.3 The Conformal Anomaly.

Conformal invariance (§2.4) can be used to extract the (bulk) critical properties from a finite system. Section 2.4.2 showed that the eigenvalues of the Hamiltonian of a strip system can be used to find the scaling dimensions of the system's operators and its conformal anomaly.

One expects to find the conformal anomaly, \( c = 1 \), since the O(2) model has a scale invariant line of criticality with continuously varying exponents. A test of the \( c = 1 \) hypothesis can be performed by calculating the exponent \( \eta \) assuming \( c = 1 \), and comparing the result with the \( \eta \) values obtained earlier in §4.3.2.1.

The results of §2.4.2 can now be applied. Equations (2.70) and (2.71) will be re-written here for convenience,

\[
\begin{align*}
F_{ij} &= \frac{A_{ij}(M)}{M} = \frac{2\pi \zeta_M x_{ij}}{M} \\
\omega_0(M) &= \epsilon' - \pi \frac{\zeta_M c}{6M^2}
\end{align*}
\]

(4.26) (4.27)

where the mass gap \( F_{ij} = \omega_j - \omega_i \), \( x_{ij} \) is the scaling dimension corresponding to the operator connecting states eigenstates \( \langle i \rangle \) and \( \langle j \rangle \) and the \( \zeta \) values at different lattices sizes have been distinguished.
Using data from pairs of lattice sizes, we can extract $\zeta_M$ from (4.27). These lattice dependent $\zeta_M$ are extrapolated to the bulk limit $\zeta$. Using (4.26), the $A_{ij}(M)$'s are determined and extrapolated to the bulk value $A_{ij}$. The $x_{ij}$ are then found from the ratio $A_{ij}/\zeta$.

The identity $2x_{01} = 2x_{23} = 2x_h = \eta$ is expected since the states $|0\rangle$ and $|1\rangle$ (and the states $|2\rangle$ and $|3\rangle$) are connected via the magnetic operator (see (2.29)). Also we expect $x_{02} = x_{13} = x_E = 2$ in the critical region as conjectured by Batchelor and Blöte (1988). The values of $2x_{01}$, $2x_{23}$, $x_{02}$ and $x_{13}$ for couplings $x = 1.8$ to $4.0$ are listed in table 4.4. From this table we can see that $2x_{01} = 2x_{23} = \eta$ as expected and for the interval $x \geq 2$ we have $x_{02} = x_{13} = 2$ within errors.

These results confirm the identification of the O(2) model as a $c = 1$ conformal system.

§4.4 Conclusion

Hamiltonian finite-size scaling methods have been applied to the (1+1)D O(2) model. Results have been extended from previous work by the study of different schemes for truncating the infinite Hilbert space of configurations into a soluble, finite subspace, by the application of the theory of conformal invariance and by the determination of the critical exponent $\eta$. A numerically efficient vector algorithm has been designed for the 'core' routine in the eigensolution package and an improved algorithm for the generation of the basis states has developed (see the appendix and §4.2.3).

The hypothesis that the O(2) model falls in conformal invariance class $c = 1$ has been demonstrated convincingly by the analysis in §4.3.3.
Conformal invariance arguments give $x_E = 2$, within errors, for the scaling dimension of the energy operator in the critical region which concurs with the conjecture made by Batchelor and Blöte (1988).

The exact position of the Kosterlitz-Thouless transition is difficult to determine accurately, due to the exponential decay of the mass gap as $x \to x_c$. The scaled mass gap method (§4.3.1.1) gives $x_c = 1.9 \pm 0.1$, the $\beta$ function fit (§4.3.1.2) gives $x_c = 2.06 \pm 0.04$, and $x_c = 2.00 \pm 0.03$ was obtained by Romberg extrapolations of the mass gap (§4.3.1.3). This uncertainty in the critical point is similar to the situation in the Euclidean version of the model (see table 4.1) where Monte Carlo estimates of $T_c$ vary by around 10%. All the evidence is in accord with the expected line of critical behaviour for $x > x_c$.

The exponent $\sigma$ in the correlation length (4.2) has been found to be $\sigma = 0.501 \pm 0.005$ using the Romany-Wyld $\beta$ function fitting procedure (§4.3.1.2), in excellent agreement with the Kosterlitz value of $\sigma = \frac{1}{2}$.

The exponent $\eta$ has been estimated as a function of coupling $x$ by finite-size scaling using the magnetization and the susceptibility (§4.3.2.1) and by conformal invariance (§4.3.3), all of which are in excellent agreement. The scaling relations $\tilde{\gamma} = 2 - \eta$ and $\tilde{\beta} = \eta/2$ have thereby been confirmed for this model. In the low temperature region, the results agree with the expected asymptotic behaviour $\eta(x) \propto x^{-1/2}$. However, near the transition point, they do not agree with the value $\eta(x_c) = \frac{1}{4}$ predicted by Kosterlitz (§4.3.2.2). This is likely to be due to logarithmic corrections to scaling, similar to those occurring in the XXZ Heisenberg model.
Chapter 5
Stochastic Truncation and the
(2+1)D $Z(2)$ Model

§5.1 Introduction

§5.1.1 The Motivation for Stochastic Truncation.

This chapter discusses a new scheme for truncating the basis set of finite-lattice Hamiltonians down to a manageable size.

In §3.2 it was shown that the number of strong coupling basis states required to span the eigenvectors accurately increases rapidly as the system moves away from the strong coupling limit. This motivated a number of deterministic truncation schemes which were tested on the lattice harmonic oscillator (§3.2) and applied to gain accurate information on the 2-dimensional $O(2)$ model in chapter 4.

As stated in §3.2 successful truncation schemes should efficiently and accurately determine the eigensolutions of finite-lattice Hamiltonians.
This chapter continues the search for efficient, accurate truncation schemes by testing a \textit{non-deterministic}, Monte Carlo style algorithm on the \((2+1)D\) \(Z(2)\) gauge model. The aim of this chapter is to test this 'stochastic truncation' algorithm itself, and not necessarily to get accurate information on the \(Z(2)\) model. The ultimate aim in all of these projects is to develop a method which can be applied to 4-dimensional gauge theories with fermions - especially quantum chromodynamics.

This work is being prepared to be published as a paper (Allton, Hamer and Yung 1988). The results of an application of stochastic truncation to a more complex model, quantum electrodynamics in 3 dimensions, is being prepared in a second paper (Yung, Hamer and Allton 1988).

\section*{5.1.2 The \((2+1)D\) \(Z(2)\) Model.}

The 3-dimensional \(Z(2)\) model is the simplest of all gauge field theories. Its lattice formalism is equivalent to the 3-dimensional Ising model under a duality transformation so its phase structure is well understood. It has a single second order critical point (with vanishing mass gap and string tension) which separates canonical high-temperature and low-temperature phases.

The lattice Hamiltonian for the model can be defined (Fradkin and Susskind 1978, Kogut 1979)

\begin{equation}
H_{\text{phys}} = \sum_l \left(1 - \sigma_l(l)\right) - x \sum_p \sigma_3(l_1) \sigma_3(l_2) \sigma_3(l_3) \sigma_3(l_4) \tag{5.1a}
\end{equation}

\begin{equation}
= H_0 - x V, \tag{5.1b}
\end{equation}

(cf. (3.1)) where \(l\) labels the links on a 2-dimensional square lattice, \(p\) the plaquettes, and the \(l_i\) are the four links which surround the plaquette \(p\). In (5.1) the Hamiltonian lattice coupling \(x\) is defined
\[ x = 1 / g^4, \]  
(5.2)

and the \( \sigma_i \) are the Pauli matrices

\[
\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.
\]  
(5.3)

The \( \mathbb{Z}(2) \) model (5.1) was chosen as a test case model for the new truncation scheme for the following reasons:

(i) It has been studied before using exact finite-lattice Hamiltonian methods (Irving and Thomas 1982, Hamer and Irving 1983).

(ii) As mentioned earlier, via a duality transformation (Fradkin and Susskind 1978), (5.1) becomes the (2+1) dimensional Ising Hamiltonian so its properties are well understood. In fact, studies of the (2+1) dimensional Ising model have provided the most accurate value of the critical point of (5.1) (Hamer and Irving 1983):

\[ x_c = 3.044 \pm 0.005 \]  
(5.4)

(iii) The finite-lattice Hilbert space is *finite*-dimensional. This means that the finite-lattice eigensolutions for small lattices can be found *exactly*, so the stochastic truncation results can be tested against these exact values. (This contrasts with the \( \mathbb{O}(2) \) model which has an *infinite*-dimensional finite-lattice Hilbert space.)

(iv) It is the simplest, non-trivial pure gauge theory.

This chapter continues with a description of the stochastic truncation algorithm, its relationship to other Hamiltonian Monte Carlo approaches and an outline of its implementation on the \( \mathbb{Z}(2) \) model. Section 5.3 contains the results of the application of the method to the \( \mathbb{Z}(2) \) model.
§5.2 Stochastic Truncation.

§5.2.1 The Method.

The stochastic truncation scheme (Hamer 1987) is a Hamiltonian Monte Carlo truncation scheme based on the power method. This section describes the method itself without any reference to application-specific numerical techniques. (Section 5.2.3 will outline the implementation of stochastic truncation to the $Z(2)$ model.)

The stochastic truncation approach is iterative in nature; at the $n$th iteration the following steps are performed:

(i) Operate $H$ on the trial ground state $|\varphi^n\rangle$. State $|\varphi^n\rangle$ is represented on a convenient basis $|I\rangle$, and has integer components $m_I^n$ in that basis:

$$H|\varphi^n\rangle = \sum_I m_I^n H|I\rangle.$$  \hfill (5.5)

(ii) Divide $H|\varphi^n\rangle$ by the 'score' $S^n$ which defines the real-valued components $c_I^{n+1}$:

$$\sum_I c_I^{n+1} |I\rangle = \frac{1}{S^n} H|\varphi^n\rangle = \sum_{IJ} \frac{H_{IJ} m_J^n}{S^n} |I\rangle,$$  \hfill (5.6)

where $S^n$ is chosen so that the 'ensemble sizes' $N_E^n$ of the trial ground states are approximately constant, that is:

$$N_E^n = \sum_I m_I^n$$  \hfill (5.7a)

$$= N_E^{n+1} = N_E^{n+2} = \ldots = constant$$  \hfill (5.7b)

One obvious definition of $S^n$ is:
\[
S^{n)} = S^{n-1)} \frac{N_E^{n)}}{N_E^{n-1)}. \tag{5.8}
\]

Other definitions of \( S^{n)} \) will be discussed in §5.3.1.

(iii) \textit{Stochastically integerize} the components \( c_l^{n+1) \) to integers \( m_l^{n+1) \) using the following scheme:

If \( r \geq \Delta, \) then \( m_l^{n+1) = [c_l^{n+1) \); \]

If \( r < \Delta, \) then \( m_l^{n+1) = [c_l^{n+1) ] + 1 . \tag{5.9b} \)

where \( r \) is a randomly chosen number between 0 and 1, \( \Delta = c_l^{n+1) - [c_l^{n+1) \] and \([z] \) is the integer part of \( z \). Obviously this will truncate from the basis set some of those states whose amplitudes \( c_l^{n+1) \) are between 0 and 1.

The \((n+1)\)th trial ground state can now be defined:

\[ |\varphi^{n+1) = \sum_I m_I^{n+1) } |I\rangle. \tag{5.10} \]

(iv) Repeat from step (i).

§5.2.2 \textbf{Relationships with Other Methods.}

Stochastic truncation is a stochastic form of the power method for finding the largest eigenvalue of a matrix. This can be readily seen if the stochastic integerizing step (step (iii) in §5.2.1) is left out, in which case, from (5.6), the \((n+1)th \) trial wavevector \( |\varphi^{n+1) \) is related to the starting vector \( |\varphi^0 \) as follows

\[ |\varphi^{n+1) = \frac{H}{S^{n)}} \frac{H}{S^{n-1)} \ldots \frac{H}{S^0) } |\varphi^0 \). \tag{5.11} \]

Equation (5.11) is simply a modified power method. Since the score \( S^{n)} \) is chosen so that ensemble size is constant and therefore \( |\varphi^{n+1) = |\varphi^n \) (for large \( n \)), we have
\[
\frac{\langle \phi^{n+1} | \phi^{n+1} \rangle}{\langle \phi^n | \phi^n \rangle} = 1, \tag{5.12}
\]
which together with (5.11) gives the estimate:

\[
\text{largest eigenvalue of } H = S^n. \tag{5.13}
\]

Stochastic truncation is also related to another scheme - the ensemble projector Monte Carlo (EPMC) method. This procedure (DeGrand and Potvin 1985) solves the eigenvalue of the operator \( u \) by generating an ensemble of states at each iteration by the operation of \( u \) on the previous ensemble. EPMC differs from stochastic truncation in that the \( m_I^n \) basis states \( |I\rangle \) in the \( n \)th ensemble are treated and stored separately, whereas in the stochastic truncation procedure this degeneracy is recognized and all the copies of the state \( |I\rangle \) in the ensemble are stored and treated together. It is worth noting that the EPMC method is a generalization of another simpler scheme, the projector Monte Carlo procedure where the ‘ensemble’ of states at each iteration consists of a single basis state \( |I\rangle \) which traces out a ‘random walk’ through the basis set \( \{|I\rangle\} \) under the operation of \( u \) (Blankenbecler and Sugar 1983).

§5.2.3 Numerical Implementation.

In applying the stochastic truncation procedure to the (2+1)D \( Z(2) \) model a few numerical/algorithmic techniques were used which were not specified in the general outline of the method in §5.2.1. The first is the choice of the basis set \( \{|I\rangle\} \). As in the \( O(2) \) project in chapter 4, the strong coupling \( (x = 0) \), symmetrized basis of (5.1) were used (see §4.2.3). This means that a very similar algorithm to that appearing in §4.2.3 steps (i) to
(iiic) is used for the operation of \( H \) on \( |\varphi^n\rangle \) (step (i) of the stochastic truncation algorithm, §5.2.1). In particular, all symmetry transformations are applied to find the representative state as in §4.2.3.

Secondly, the starting vector \( |\varphi^0\rangle \) was chosen to be the strong coupling ground state \( |0\rangle_{x=0} = |0\rangle \) as all that is required of \( |\varphi^0\rangle \) is that it have some overlap with the desired symmetry sector. The choice of \( |\varphi^0\rangle \) can be optimized to lie close to the true ground state but since this would require information about the basis states in advance, and since the equilibration time is short in this application this is not necessary.

The third numerical technique specific to the \( \mathbb{Z}(2) \) model was the way in which the representative states \( |\uparrow;1\rangle \) themselves are stored (see §4.2.3). A 'plaquette' representation was found most efficient where each plaquette \( p \) on the lattice is represented by a single memory bit which is set to 0 (1) if the plaquette operator \( \sigma_3(l_1) \sigma_3(l_2) \sigma_3(l_3) \sigma_3(l_4) \) has acted on \( p \) an even (odd) number of times. This representation saves a factor of 2 in storage compared with the alternative 'link' representation where each bit stores the state of a link.

Finally, in order to apply the stochastic truncation method to find the lowest eigensolution of \( H_{\text{phys}} \) (5.1), the following operator must be used in the stochastic truncation routine:

\[
H = E_{\text{max}} - H_{\text{phys}}. \quad (5.14)
\]

This introduces the parameter \( E_{\text{max}} \). Fortunately the efficiency of the routine is not critically affected unless \( E_{\text{max}} \) is chosen to be very small, in which case the scheme iterates towards \( |E_{\text{max}} - \omega_{\text{max}}| \) where \( \omega_{\text{max}} \) is the largest eigenvalue of \( H_{\text{phys}} \). (If \( E_{\text{max}} \) is chosen to be very large then the equilibration time is lengthened.)
§5.3 Results

§5.3.1 Definitions for the Score $S^n$.

All that is required of the score $S^n$ is that it keep the ensemble size constant (see (5.7b)), so there are obviously a number of ways of defining it. In §5.2.1, one possible definition for the Score $S^n$ was given in (5.8). When this 'naive' choice was used to define $S^n$, neighbouring scores $S^n$ and $S^{n+1}$ (generally) were found to be anti -correlated. That is, on average, $S^n$ and $S^{n+1}$ are on opposite sides of the average score $\langle S^n \rangle$. This is exhibited in figure 5.1 where the correlation function $c(n)$ is plotted for a 4x4 lattice. ($c(n)$ has the usual definition: $c(n) = \Sigma_m (S^m) - \langle S^1 \rangle (S^{m+n}) - \langle S^1 \rangle$ with the sum over the equilibrium region.)

![Correlation Function](image)

Figure 5.1 The correlation function defined in §5.3.1 for the naive score definition. The run was made on a 4x4 lattice in the vacuum sector at $x = 2$. The initial ensemble size $N_0^{(0)}$ was 1000.
Obviously this (anti-)correlation reduces the number of independent
iteration steps and is thus an undesirable feature. An attempt was made
to average out the anti-correlation by defining the score to be

\[ S^n = aS^{n-1} + (1 - a) S^{n-1} \frac{N^n}{N^{n-1}}, \tag{5.15} \]

where \( a \in [0,1] \). This definition for \( S^n \) is a weighted average between the
the naive definition (5.8) and the score of the previous step \( S^{n-1} \).

The naive score definition (5.8) and the definition (5.15) were applied
to a test lattice to see which gave the least statistical error \( \sigma(S^n) \). In defining
the statistical error, the method of blocking described in Binder
(1976) was followed in which averages \( \langle S^n \rangle_v \) of ‘blocks’ \( v \) \( (v = 1,2, \ldots) \)
were formed for different size blocks. The standard error in these block
averages is then a constant for all block sizes \( N' \), so long as \( N' \) is greater
than the correlation length of the raw data, and the number of blocks is
statistically large. This constant value is then used as the estimate of the
statistical error in the average score \( \langle S^n \rangle \).

The definition for \( S^n \), (5.15), gave only a slightly lower value for the
statistical error than the naive definition (5.8) (even for the ‘best’ value of
\( a \)). Because the improvement in accuracy was only small, and since in
any case the best value for \( a \) cannot be determined \textit{a priori}, the naive defi-
nition is the favoured one.

There are many other possible definitions for the score \( S^n \) besides
the two mentioned already. A number of these were tested, the most ac-
curate, \( S^n = S^{n-1} \sqrt{\langle I \rangle / N^{n-1}} \), giving a statistical error around ten
times smaller than the naive definition. However, this definition did not
always give convergence and so was discarded!
As the results of these tests favour the choice of (5.8) for the definition of the score it will be used from here on. (Other applications of stochastic truncation may find other definitions more suitable.)

§5.3.2 Estimates of the Errors.

As is generally true in Monte Carlo investigations, there are three sources of errors which affect the calculation: equilibration errors (caused by measurements on a system not yet in equilibrium); statistical errors; and systematic errors. Each of these sources of error will be discussed in turn.

Figure 5.2 The eigenvalue estimate against step number for the ground state in the vacuum sector for a 4x4 lattice at \( x = 3 \). This plot shows the number of steps required to reach equilibrium is small, even close to the critical point. The dotted line is at the eigenvalue averaged over the region from the 100th to 1000th iteration.
(i) Equilibration Errors. In all cases studied (for lattices up to 4×4's and with couplings in the range \( x = 0 \rightarrow 3 \)), equilibrium was rapidly reached well within the hundredth step even for couplings close to the critical point \( x_c = 3.044 \). This is demonstrated in figure 5.2 where the eigenvalue estimates of \( H_{\text{phys}} \) (obtained from the scores using (5.13) and (5.14)) are plotted against step number for a 4×4 lattice at coupling \( x = 3 \).

As expected from other Monte Carlo simulations, the equilibration time is greatest for couplings close to the critical point.

(ii) Statistical Errors. (The method for determining the statistical errors has been explained in the previous subsection.)

Statistical errors were found to decrease as \( \frac{1}{\sqrt{N_I}} \) where \( N_I \) is the number of iterations in the equilibrium region. This is the expected statistical behaviour and confirms the validity of the method for estimating the statistical error.

As well as the variation with \( N_I \), the statistical error is expected to fall as the ensemble size increases. This behaviour for a 4×4 lattice at coupling \( x = 2 \) is shown in figure 5.3 where the logarithm of the statistical error is plotted against the logarithm of the average ensemble size in the equilibrium region \( \langle N_{E^n} \rangle \). As can be seen from the figure, a behaviour: statistical error \( \sim \frac{1}{\langle N_{E^n} \rangle} \) ; (for the ensemble sizes shown) is obtained.

This can be understood by the following. Due to the stochastic integerization, the basis state amplitudes \( \langle \psi^n \mid \phi^n \rangle \) differ from the true value by an amount \( \sim O(1) \). The relative error in these amplitudes will be thus \( O(1/N_E) \). When the scores defined in (5.8) are used to estimate the eigenvalues (using (5.13)) we have
nth eigenvalue estimate = \( S^n = S^{n-1} \frac{N_E^n}{N_E^{n-1}} = \frac{\langle \chi | H | \varphi^{n-1} \rangle}{\langle \chi | \varphi^{n-1} \rangle} \) (5.16)

where the state \( |\chi\rangle \) is the 'broad' state \( \Sigma_I |I\rangle \). Using (5.16) the relative error in the eigenvalue estimate can be shown to be proportional to the relative error in the amplitudes \( \langle I | \varphi^n \rangle \) and hence of order \( \frac{1}{\sqrt{N_E}} \) as observed. (For more extreme cases where the ensemble size is small compared with the dimension of the basis set and the average of the state's amplitudes is less than one, the above argument will fall down and a different behaviour for the statistical error will be expected.)

**Figure 5.3** A plot of the log of the statistical error against the log of the average ensemble size \( N_E \) (base 10). A 4x4 lattice was used at \( x = 2 \) in the vacuum sector. This plot shows a \( \frac{1}{N_E} \) behaviour for the statistical error.
(iii) **Systematic Errors.** Using (5.16) it can be shown that the 'exact' error \( \omega_{\text{exact}} - \langle S^n \rangle \) can take both signs. This difference was calculated numerically using the exact Hamiltonian eigenvalues for various lattice sizes and couplings and indeed it was found to have both positive and negative signs, apparently at random. Thus there is no evidence for any systematic error in the stochastic truncation eigenvalue estimates from these results.

The numerical values of the exact error were of the order of the statistical error, except for the 'large' lattice size (ie. 4x4) when the coupling was greater than \( \sim 2.5 \). Although it is known from all other approaches that the critical region is difficult to study accurately, no precise explanation of this behaviour has been derived.

§5.3.3 **Eigenvalue Estimates and Scaling.**

Estimates for the lowest energies in the vacuum and axial string sector, \( \omega_0 \) and \( \omega_1 \), were obtained for the 2x2, 3x3 and 4x4 lattices for \( x = 0.5, 1.0, \ldots, 3.0 \) using a 1000 step run. A plot of the ground state energy estimate per site for the vacuum sector is shown in figure 5.4.

The finite-lattice axial string tension \( T_a(M,x) \) is plotted in figure 5.5 for \( M \times M = 2 \times 2, 3 \times 3 \) and \( 4 \times 4 \) lattices where (Hamer and Irving 1983)

\[
T_a(M,x) = \frac{\omega_1(M,x) - \omega_0(M,x)}{M} .
\]

(5.17)

The statistical error in all of the curves in figures 5.4 and 5.5 is below the resolution of the graphs (of the order of \( 10^{-5} \), \( 10^{-4} \) and \( 10^{-2} \) for the 2x2, 3x3 and 4x4 lattices respectively). The 'exact' error, \( \text{exact} - \langle \text{estimate} \rangle \), is similarly below the resolution of the graphs, except for the axial string tension curve for the 4x4 lattice at \( x=3 \) where it is represented as an error bar.
Figure 5.4 Estimate of $\omega_0 / M^2$ from stochastic truncation against coupling $x$ for lattice sizes $MxM = 2x2, 3x3$ and $4x4$. (Following Hamer and Irving 1983, fig. 2a.) The program ran for 1000 iterations and equilibrium was assumed to be reached at the 100th step. The errors in these curves, both statistical and 'exact', are too small to be shown.

Figure 5.5 Estimate of the axial string tension (following Hamer and Irving 1983, fig. 5a). The run was set up as in figure 5.4. All errors are too small to be indicated except for the $4x4$ where the 'exact' error (the difference between the estimated and exact string tension) is indicated as an error bar for $x = 3.0$. 
It is clear that the data is accurate enough to obtain an estimate of $x_c$ from the scaling behaviour. This procedure was not carried out since the aim was to test the stochastic truncation method itself and not to gain accurate information on the model's critical behaviour. (Also, by definition, the exact finite-lattice method will be more accurate!)

§5.4 Conclusion.

The stochastic truncation method has been shown to converge towards the correct eigenstates for the (2+1)D $Z(2)$ gauge model, and has thus been shown to be a successful Hamiltonian Monte Carlo scheme. Importantly, this convergence was maintained even in the critical region.

Various definitions for the 'score' were studied with the result that accurate convergence can be hindered by a badly chosen definition. The scheme showed no evidence of systematic errors. The statistical error, obtained from the 'blocked averaging' technique was found to fall as $1/N_E$ where $N_E$ is the (average) ensemble size in the equilibrium region.

In a 'production run' of 1000 steps (ie. 1000 operations of $H$), accurate eigenvalues were obtained. This compares unfavourably with the exact finite-lattice method which obtains machine precision results with less than 100 operations of $H$. Furthermore, the stochastic method calculates $H_{I,J}$ a-fresh at each step whereas the exact method defines $H_{I,J}$ once only.

The stochastic truncation method is expected to compare favourably with the exact finite-lattice approach for 4-dimensional theories where the exact approach fails for even small lattice sizes due to the exponential growth of basis states. The main advantage of stochastic truncation is that it selects the most important subspace in a natural way as it goes.
Chapter 6

Conclusion

"I want to be there when everyone suddenly finds out what it has all been for."
- Fyodor Dostoyevsky.

§6.1 Summary of the Projects.

In chapters 2 and 3 the two halves of the Hamiltonian finite-lattice approach were discussed separately. The first half, that of finding the lowest eigensolutions of the Hamiltonian operator represented on an appropriate basis, was discussed in chapter 3. This included the testing of four deterministic basis state truncation schemes on the lattice harmonic oscillator to see which was the most accurate and efficient. Matrix eigensolution routines were discussed and the N-step Lanczos procedure introduced.

Chapter 2 overviewed finite-size scaling and conformal invariance which are the tools that can be used to find the bulk critical behaviour from the analysis of a finite portion of the system. These tools were ‘derived’ using a renormalization group framework based upon the correlation function transformation law.
In chapter 4, a detailed study of the (2+1) dimensional O(2) or planar rotator model was described. This project further tested the truncation schemes found to be most effective in chapter 3. The result was that the energy cut-off scheme is the most accurate and efficient. The 'production runs' used the N-step Lanczos routine, and the eigensolutions were obtained up to a 9-site lattice. An algorithm was developed for the 'core' routine of sparse matrix multiplication which can be written as a vectorized code. Both finite-size scaling and conformal invariance were used to gain estimates of the bulk properties.

Three methods of predicting the critical point all gave $x_c \approx 2.0$ (see §4.3.1). The small size of the error in some of these predictions leads to the conjecture that $x_c = 2$ exactly. Also the equivalence of the Hamiltonian strong coupling and Euclidean high temperature expansions for the critical exponent $\eta$ using the 'naive' relation $x = 2/g^2 = 2/\tau^2$ leads to the conjecture $\tau_c = kT_c /J = 1$ for the Euclidean critical point.

The conformal anomaly of the system was confirmed to be $c = 1$ by the first application of conformal invariance to the model. The scaling dimension of the energy operator was shown to be $x_E = 2.0$ for the critical region $x \geq x_c$.

The exponent $\sigma$ governing the exponential divergence of the correlation length has been found to agree with the Kosterlitz value $\sigma = 1/2$. The magnetic exponent $\eta (= 2x_h)$ was derived as a function of coupling but the exact result $\eta_c = 1/4$ (Batchelor and Blöte 1988) was not observed. The discrepancy can be explained by possible logarithmic corrections to scaling similar to those known to occur in other models with a Kosterlitz-Thouless transition.
The hexagonal-lattice O(2) invariant model with the simplified partition function (4.3) (which is exactly soluble at its critical point) has been shown in appendix A to correspond to the same Hamiltonian as the canonical O(2) partition function (4.1) (ie. (4.4)).

It is difficult to see how a more accurate determination of the O(2) model's critical behaviour can be made using the finite-lattice Hamiltonian approach unless more computing power is applied, particularly since the transition is so subtle. The strong-coupling basis is the natural choice for lattice Hamiltonian work which unfortunately leads immediately to the problem of huge matrices in order to obtain the ground state accurately. There have been many truncation schemes tested to contain this problem by several workers in the field (and in this dissertation), and, although some improvements can be made over the most basic schemes, it appears deterministic, strong-coupling basis schemes (modestly!) are at their limit. Applying the best of these basis state truncation schemes to finite-lattice Hamiltonians still leaves very large matrices (for accurate solutions). For example, the 9-site lattice data in the O(2) project for $x \geq 2$ could not be used since the matrix size needed to get accurate eigensolutions in this region was impossibly large. The conclusion is then, for the type of approach used in chapter 4 (ie. deterministic with a strong-coupling basis), an increase in computer power is a necessity for any further increase in accuracy, particularly for systems with 3 or more dimensions. More on the prospects for advancement using other approaches will be given in the next section.

The limits of the deterministic approach to the problem and the success of Monte Carlo approaches in Euclidean statistical mechanics motiva-
ted the proposal of a stochastic style truncation scheme for Hamiltonian problems (Hamer 1987). This 'stochastic truncation' scheme chooses the most important strong-coupling states $|I\rangle$ (ie. those with largest amplitude $\langle I|0 \rangle$) in a stochastic manner by integerizing the basis state amplitudes. The method is a 'Monte Carlo' style power method and is similar to the ensemble projector Monte Carlo approach.

Stochastic truncation was tested on the (2+1) dimensional $Z(2)$ model and was found to give accurate results, but only after a great deal of CPU time. Various definitions for the 'Score' $S^n$ were studied and the best was used in some 'production runs' to determine the lowest eigenvalues of the system. The method's statistical properties were studied; there was no evidence for any systematic error and the statistical error's behaviour as a function of 'ensemble size' $N_E$ was mapped out. The eigenvalues were found for a number lattice sizes up to the 'medium' sized 4×4 and these were used to find the finite lattice axial string tension.

While stochastic truncation is not the most efficient method in this 3-dimensional model due to the large number of operations of the Hamiltonian required (the exact finite-lattice method needs far fewer - and for exact results), it may prove useful in 4-dimensional theories where the exact finite-lattice method is stalled on even very small lattice sizes.

§6.2 Future Directions.

Prospects for a more accurate determination of lattice theories' critical behaviour using a Hamiltonian finite-lattice approach await advancement in two areas: computing power and the method of solution. These two issues will be dealt with here in turn.
Computational physics fields, such as lattice gauge theory, are limited in the physics they can study by the contemporary crop of computers. This situation is identical to that faced by experimentalists, particularly particle physicists, who are constrained by the energies of their accelerators. Inevitably, more powerful machines will be built to satisfy the curiosity of the scientists! A laissez-faire approach to lattice gauge theory is thus possible, in which one awaits evermore powerful machines (a desktop CRAY III perhaps?).

An alternative approach to the field, as with experimental high energy physics, is through the re-thinking of the method of attack. The success of this approach is unpredictable compared with relying on a few more gigaflops, but some of the conclusions of the work so far are certain to act as a guide. The successes of most of the techniques applied so far can be summarized by: the simpler, the faster, the better. The truncation schemes tested on the lattice harmonic oscillator in §3.2 in particular support this statement. Applying this to the Hamiltonian approaches taken so far is not encouraging. It is hard to envisage a simpler deterministic truncation scheme than the energy cut-off method applied to the strong-coupling states, or a simpler Hamiltonian Monte Carlo technique than stochastic truncation!

Perhaps following the success of hybrid, Euclidean, Monte Carlo schemes where, for example, molecular dynamics and the heat bath algorithms are applied serially, a hybrid Hamiltonian scheme could be devised. Combinations that come to mind include: (i) using weak and strong coupling basis states in turn to iterate towards a solution; (ii) a stochastic Lanczos algorithm (after all stochastic truncation is based on the power
method which is a very inefficient way of eigensolving); or (iii) some combination of stochastic and deterministic schemes.

Leaving aside the finite-lattice Hamiltonian approach in its generalities, some more specific directions for future research include deriving the second term in the $\eta(x)$ and $\eta(\tau)$ expansions for the O(2) model to see if they are equal using the 'naive' equivalence $x = 2/\tau^2$. This would add weight to the conjecture $\tau_c = 1$. It would also be interesting to try to follow a 'critical path' in coupling space $(K_xK_y)$ to see if it is parameterized by $K_xK_y = 1$. 
Appendix A

Hamiltonian Form of Nienhuis' O(2) Symmetric Partition Function

Nienhuis (1982) studied an O(2) symmetric model with partition function

\[ Z = \prod_{\text{sites } k} \left\{ \int d\vec{s}(\vec{r}_k) \right\} \prod_{\langle ij \rangle} \left[ 1 + x \vec{s}(\vec{r}_i) \cdot \vec{s}(\vec{r}_j) \right] , \quad (A.1) \]

where the second product is over nearest-neighbours \( \vec{r}_i \) and \( \vec{r}_j \) on a hexagonal lattice and the \( \vec{s}(\vec{r}) \) are n-component spins of unit length. Nienhuis' work and that of Baxter (1986) and Batchelor and Blöte (1988) have been discussed in §4.1.2. In this appendix the Hamiltonian corresponding to (A.1) is derived and found to be the 'canonical' (1+1)D O(2) Hamiltonian (4.4). Thus the change in the form of the partition function between (4.1) and (A.1) and the hexagonal rather than rectangular lattice doesn't alter the (time continuum) Hamiltonian formalism. While this is expected from universality arguments it is interesting that the two models can be proved to be in the same universality class in this manner.

The method described below can be generalized to other symmetries and other non-square regular lattices.

We begin by recalling that the classical Hamiltonian \( \mathcal{H} \) (see table 1.1) can be defined from the partition function
Recognizing the multiple integral in (A.1) as an integral over configurations, the classical Hamiltonian of (A.1) can be defined

\[ \mathcal{H} = - \sum_{\langle ij \rangle} \ln[1 + x s(r_i) \cdot s(r_j)]. \quad (A.3) \]

The sum is over nearest neighbours on a hexagonal lattice which can be represented as in figure A.1 (see Baxter 1986). There are three bond types on the lattice, and, following Fradkin and Susskind (1978), we will distinguish between them. The lattice spacings and couplings along each bond type will be defined \( a_i \) and \( K_i \), \( (i = x,y,t) \). The classical Hamiltonian (A.3) can now be written (where the \( a_i^\uparrow \) have an obvious definition)

\[ \mathcal{H} = - \sum_{\text{circled } \vec{r}} \{ \ln[1 + K_x \vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_x)] \\
+ \ln[1 + K_y \vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_y)] \}
+ \ln[1 + K_t \vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_t)] \] 

---

**Figure A.1** The hexagonal lattice with the three bond types \( x, y \) and \( t \) displayed. The circled sites appear in the sum in (A.4).
Fradkin and Susskind discuss the time-continuum limit of the canonical $O(2)$ model in which the time-like coupling becomes infinite (correlating the spins along that direction), the time-like lattice spacing shrinks to zero and the space-like coupling becomes infinitesimal. In this 'extreme anisotropic' limit the time-like columns of spins are driven to the trivial critical point. For the hexagonal lattice, figure A.1, there are two time-like couplings. We are free to take their limits $K_t, K_y \to \infty$ and $a_t$, $a_y \to \infty$ so that $K_y \gg K_t$ and $a_y \ll a_t$. This will 'freeze' the spins connected by a 'y' bond, and the classical Hamiltonian (A.4) becomes

$$\mathcal{H} = -\sum_i \{ \ln[1 + K_x \vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_x)] + \ln[1 + K_t \vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_t)] \}$$

(ignoring an irrelevant constant). The sum is effectively over a rectangular lattice so the hexagonal nature of the lattice has disappeared. Continuing with the extreme anisotropic limit $\mathcal{H}$ can be simplified to

$$\mathcal{H} = -\frac{1}{a_t} \int dt \sum_x \{ K_x \vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_x) - \frac{1}{2} \left[ a_t \nabla_t \vec{s}(\vec{r}) \right]^2 \}$$

again ignoring constants and using $K_x \to 0$, $K_t \to \infty$ and $a_t \to 0$ (so we have $\vec{s}(\vec{r}) \cdot \vec{s}(\vec{r} + \vec{a}_t) = 1 - \frac{1}{2} \left[ \vec{s}(\vec{r}) - \vec{s}(\vec{r} + \vec{a}_t) \right]^2 \to 1 - \frac{1}{2} \left[ a_t \nabla_t \vec{s}(\vec{r}) \right]^2$). Note that for both the 'x' and 't' terms in $\mathcal{H}$ to be of the same order, the extreme anisotropic limit should be taken so that $K_x = a_t^2$.

We now confine our interest to the case $n = 2$. We can follow Fradkin and Susskind directly since their equation (4.7) is identical to (A.6) with their coupling parameter $\lambda = K_x / a_t^2$. The quantum Hamiltonian corresponding to (A.1) is thus (4.4). Unfortunately, since only the isotropic critical Neinhuis model was solved (Baxter 1986) the critical point of the Hamiltonian version of the model cannot be extracted from this procedure.
Appendix B

'Knitting' Algorithm for Sparse Matrix Multiplication

The following outlines a fully vectorized code which multiplies a sparse matrix by a vector. The code was used in the N-step Lanczos procedure in the O(2) project where the Hamiltonian matrix is multiplied by a Lanczos vector (step(ii), §3.3). It was designed to run on a Cyber 205 vector supercomputer.

The aim is to use vector instructions which manipulate long vectors to find \( \mathbf{B} \) where

\[
\mathbf{B} = \mathbf{H} \mathbf{A},
\]

\( \mathbf{H} \) is a sparse matrix, and \( \mathbf{A} \) and \( \mathbf{B} \) are vectors. We will only be interested in the off-diagonal elements of \( \mathbf{H} \) since the diagonal ones are easily dealt with in a vector code.

Before the code itself is described, the following arrays are defined which contain the matrix \( H_{i,j} \):

\[
\text{MXEL}(S) = < J | V | I >, \quad \text{where the matrix elements are stored row by row as } S \text{ increases (only non-zero matrix elements are stored). The order that the matrix elements are stored within each row is unimportant.}
\]

\[
\text{COL}(S) = J, \quad \text{where } \text{MXEL}(S) = < J | V | I >, \quad \text{(ie. it is the column index for the element MXEL}(S)).
\]
\[ \text{ROW}(I) = S, \] where the first element of the \( I \)th row of \( H_{I,J} \) to appear in the \textit{MXEL} array is \textit{MXEL}(S) (i.e. it is a pointer to the start of the \( I \)th row parcel in \textit{MXEL}(S)).

Throughout this appendix, the array addresses \( S \) and \( I \) take the following values

\[ S = 1,2,\ldots,N_{\text{MXEL}} \quad (B.2a) \]
\[ I = 1,2,\ldots,N_{\text{states}}. \quad (B.2b) \]

where \( N_{\text{MXEL}} \) is the number of non-zero matrix elements, and \( N_{\text{states}} \) is the dimension of \( H \).

A fully vectorized code for (B.1) can be defined as follows :-

(i) \[ \text{DUMMYA}(S) = A(\text{COL}(S)); \quad S = 1,\ldots,N_{\text{MXEL}} \]

This distributes the components of \( A \) throughout \textit{DUMMYA} so that their order coincides with the \textit{MXEL} array.

(ii) \[ \text{DUMMYA}(S) = \text{MXEL}(S) \ast \text{DUMMYA}(S); \quad S = 1,\ldots,N_{\text{MXEL}} \]

This carries out the matrix multiplication element by element.

One can now picture pushing the \textit{DUMMYA} elements to the left side of the matrix (maintaining their rows) so that all that remains to do is add up the elements along the \( I \)th row and place the result into \( A(I) \).

(iii) \[ \text{DO} \ (v) \quad J' = 1,2,\ldots,N_{\text{local opr}} \]

\( J' \) here is a 'column' index, and \( N_{\text{local opr}} \) is the number of local operators applied in step (iiia) of §4.2.3. (The number of non-zero elements in each row of \( H_{I,J} \) is at most \( N_{\text{local opr}} \).)

(iv) \[ \text{SILLYB}(I) = \text{DUMMYA}(\text{ROW}(I) + J' - 1); \quad I = 1,\ldots,N_{\text{states}} \]

This gathers the \( J' \)th (non-zero) combination \( H_{I,J}A_J \) along row \( I \).

(v) \[ \text{WHERE} (\text{ROW}(I) + J' - 1 < \text{ROW}(I+1)) \]
\[ B(I) = B(I) + \text{SILLY}B(I); \ I = 1, \ldots, N_{\text{states}} \]

This accumulates \( B(I) \) by adding the \( J \)th non-zero 'column' of \( H_{I,J} A_J \) to \( B(I) \). The WHERE statement takes care of rows which contain less than \( N_{\text{local opr}} \) non-zero elements.

Each of the above statements (i) \( \rightarrow \) (v) takes one line of vector FORTRAN. In particular, the statements (i) and (iv) can be coded using the 205's intrinsic and very efficient 'gather' function.

The actual code used included the 'blocking' technique (see the appendix of Hamer and Johnson 1986) which breaks the matrix up into blocks small enough to fit in the main memory of the machine. This is designed to decrease page faulting which occurs when the calculation involves memory elements outside the main memory.

The above code in 'production runs' on a 205 was 300 times faster than on a DEC Vax780 computer. The speed-up factor for the whole \( N \)-step Lanczos matrix eigensolution algorithm (box §3.3, figure 3.1) was 400 which is equal to the ratio of the raw MFLOPS ratings of the two machines.


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