MONTE-CARLO SIMULATION STUDY OF PROBLEMS OF QUANTUM FIELD THEORY AND CRITICAL PHENOMENA

by

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A Dissertation Submitted to the Faculty of the

DEPARTMENT OF PHYSICS

In Partial Fulfillment of the Requirements
For the Degree of

Doctor of Philosophy

In the Graduate College

THE UNIVERSITY OF ARIZONA

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THE UNIVERSITY OF ARIZONA
GRADUATE COLLEGE

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ACKNOWLEDGEMENTS

I would like to thank Prof. Adrian Patrascioiu for his guidance and help throughout all stages of my graduate research.

Thanks are due to my friends and colleagues Mr. Ghi-Ryang Shin, Dr. Tugrul Hakioglu, Mr. Jangjin Chae, Mr. Jaeshin Lee, Mr. Ki-Dong Oh and Dr. Lowell D. Lamb, who helped me with computer work.

Also, I must thank my wife Hyunsue, who has given me so much support.

Our numerical computations were made on CONVEX C240 and IBM 3090 300E at the university of Arizona.

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ABSTRACT

In chapter one, we explain briefly the continuum limit, scaling, and high temperature expansion of critical phenomena, Monte Carlo algorithms and fitting.

In chapter two, different continuum limits of the Ising model in dimensions (D) 2, 3 and 4 are investigated numerically. The data indicate that triviality occurs for $D = 4$ and fails for $D < 4$ in each limit.

In chapter three, a relation between the critical exponents of the leading and confluent scaling terms is derived using the finite size scaling argument. We also determine the new scaling variable of the 4D Ising model based on a new Monte Carlo simulation data.

In chapter four, a Monte Carlo study of two dimensional diluted Ising systems is reported. It is shown that regular dilution does not affect critical exponents, while a random one does, with critical exponents varying continuously with impurity concentration. The importance of fluctuations in producing such effects is emphasized.

In chapter five, a different point of view regarding the critical exponent of the specific heat of the 3D Ising model is presented. Based on the analysis of high temperature expansion, finite size scaling and Monte Carlo data in the symmetric phase of the 3D Ising model, it is shown that logarithmic scaling behavior of specific heat is more consistent than power scaling behavior.

CHAPTER 1

GENERAL INTRODUCTION AND METHODOLOGY

1.1 Lattice Model as a Continuum Limit

With Feynman's path integral quantization, the ϕ^4 theory in Euclidean space is described by its Schwinger functions,

$$S_n(x_0, \ldots, x_n) \equiv < \phi(x_0) \ldots \phi(x_n) >, \tag{1.1}$$

which is averaged with respect to the *formal* measure

$$\prod_{x \in \mathbf{R}^4} d\phi(x) \exp[-S_E[\phi(x)], \tag{1.2}$$

$$S_E[\phi(x)] = \exp\{-\int \left(\tfrac{1}{2}|\nabla\phi(x)|^2 + \tfrac{m^2}{2}\phi(x)^2 + \tfrac{\lambda}{4!}\phi(x)^4\right) dx\}. \tag{1.3}$$

Except for the Gaussian case where λ is zero, this integration is not defined in general. The only analytically accessible method is perturbation theory, where the Euclidean action is a sum of Gaussian action and a small perturbation. In this case, the exponential of the small perturbation can be Taylor expanded, and the integration can be done analytically. Since the main contributions to the Schwinger function come from the configurations of $\phi(x)$ which make the Gaussian action minimum, and from slight fluctuations around that minimum, the result of perturbative calculations can be correct only when the large fluctuations around the minimum are suppressed for some physical reasons; the result of perturbation theory would not be reliable otherwise.

One way to define the integral (1.2) would be by introducing a *discrete* lattice. On a lattice the matter field is defined only on the lattice sites, and

fluctuations of the field between adjacent sites will be ignored. In this sense, introducing a lattice is equivalent to replacing $\mathbf{R}^4$ in eq(1.2) with $a\mathbf{Z}^4$, where a is a certain positive number. So it is evident that as the lattice becomes denser and denser, meaning that the length between two adjacent sites (a) approaches zero, all the configurations of the field contribute to the Schwinger functions: this limit will be called the continuum limit. We always consider the physical situation where the fields separated by a finite distance are correlated. When $a \to 0$, a finite distance in *physical units* is equivalent to an infinite length in the lattice unit (in units of a), so that it can be said that the continuum limit is obtained when the corresponding lattice model has infinite correlation length (CL). In statistical physics at the critical point CL becomes singular, so that the continuum limit of a quantum field theory will be obtained as one approaches the critical point of the corresponding lattice model. In general, there are two approaches to the critical point (or to the critical line): one in the symmetric phase where the symmetry of the original system is manifest, the other in the phase where the symmetry is spontaneously broken.

In order to illustrate the relation between a quantum field theory and the corresponding statistical model, let us note that after a rescaling of the field,

$$\phi = Const. \times \bar{\phi}, \tag{1.4}$$

S_E can be rewritten as

$$S_E = -\kappa \sum_{n\mu} 2\bar{\phi}_n \bar{\phi}_{n+\mu} + \sum_n \bar{\phi}_n{}^2 + \lambda' \sum_n (\bar{\phi}_n{}^2 - 1)^2, \tag{1.5}$$

where

$$\phi = \sqrt{2\kappa}\bar{\phi} \tag{1.6}$$

$$\lambda = 6\lambda'/\kappa^2 \tag{1.7}$$

$$m^2 = (1 - 2\lambda - 8\kappa)/\kappa \tag{1.8}$$

Here we set $a = 1$. Now, consider the model in the limit

$$\lambda \to \infty, \quad \kappa \text{ fixed}. \tag{1.9}$$

The factor in the action 1.5

$$exp\{-\lambda'(\bar{\phi_n}^2 - 1)^2\} \tag{1.10}$$

vanishes in this limit unless $\bar{\phi_n}^2 = 1$, which means that only $\bar{\phi_n} = \pm 1$ contribute to the Schwinger functions. This shows that the lattice ϕ^4 theory, in the limit where the bare coupling constant becomes very large, is the Ising model whose partition function is defined as follows:

$$Z = \sum_{n,\mu} \exp\{-\beta\sigma_n\sigma_{n+\mu}\}. \tag{1.11}$$

Here σ_n is a spin on the lattice site n, and it is either 1 or -1. In this parlance, it is evident that 2κ plays the same role as the inverse temperature β in the limit $\lambda' \to \infty$.

The relation between Ising model and lattice ϕ^4 is deeper than this. To illustrate this point, note that identity [1]

$$\int_{-\infty}^{\infty} \prod_{k=1}^{N} dx_k \exp\left(-\frac{1}{4}x_i J_{ij}^{-1} x_j + s_i x_i\right) = Const. \times \exp(s_i J_{ij} s_j) \tag{1.12}$$

where J is any symmetric positive definite matrix, and summation on the repeated indices is implied. Thus the generalized partition function of the Ising model in the presence of a magnetic field H can be written as:

$$\begin{aligned} Z\{H_i\} &= \sum_{s_i} exp(s_i J_{ij} s_j + H_i s_i) && (1.13) \\ &= \int_{-\infty}^{\infty} \prod_{i=1}^{N} d\psi_i \exp[-\frac{1}{4}\psi_i J_{ij}^{-1}\psi_j + (\psi_i + H_i)s_i] && (1.14) \\ &= \int_{-\infty}^{\infty} \prod_{i=1}^{N} d\psi_i \exp[-\frac{1}{4}(\psi_i - H_i)J_{ij}^{-1}(\psi_j - H_j)] \times \sum_{s_i} \exp(\psi_i s_i) && (1.15) \end{aligned}$$

Making use of

$$\sum_{s_i} = \prod_i (2\cosh\phi_i) = Cons. \times \exp\{\sum_i \ln(\cosh\phi_i)\} \tag{1.16}$$

and

$$\phi_i \equiv \frac{1}{2} J_{ij}^{-1} \psi_j, \tag{1.17}$$

we obtain

$$Z\{H_i\} \propto \exp\left(-\frac{1}{4} H_i J_{ij}^{-1} H_j\right) \tag{1.18}$$

$$\times \int D\phi \exp\{-\phi_i J_{ij}^{-1} \phi_j + H_i \phi_i + \sum_i \ln[\cosh(2J_{ij}\phi_j)]\}. \tag{1.19}$$

This relation shows that a certain scalar field theory corresponds to the Ising model.

In this dissertation we will focus mainly on the study of the continuum limit of the ϕ^4 theory in the limit $\lambda \to \infty$, which is equivalent to the study of the Ising model.

1.2 Various Definitions of Physical Quantities

In many cases, physically interesting quantities are related with the so called connected n-point function, which will be denoted as

$$G(x_1, \ldots, x_n) \equiv < (\phi(x_1) - < \phi(0) >) \cdots (\phi(x_n) - < \phi(0) >) >_c , \tag{1.20}$$

and the Fourier conjugate of $G(x_1, x_2)$, which will be denoted as

$$\tilde{G}(p) \equiv \sum_x e^{ip \cdot x} G(0, x). \tag{1.21}$$

For the ferromagnetic Ising model with the Hamiltonian

$$H = -\sum_{<i,j>} \sigma_i \sigma_j, \tag{1.22}$$

$$\chi \equiv \sum_x < (\sigma_0 - < \sigma_0 >)(\sigma_x - < \sigma_0 >) >_c = \tilde{G}(p = 0). \tag{1.23}$$

Using translation invariance, χ can be written as

$$\chi = \frac{1}{L^D}(< S^2 > - < S >^2) \tag{1.24}$$

where

$$S = \sum_i \sigma_i. \tag{1.25}$$

The above eq(1.24) shows that the magnetic susceptibility is proportional to the statistical fluctuations of the total magnetization of the system. In a similar way, specific heat per link is proportional to the fluctuations of the energy of the system,

$$C_v \equiv \beta^2(< H^2 > - < H >^2)/L^D/D. \tag{1.26}$$

The fact that these quantities grow to infinity approaching the critical point means that in this limit any kind of configuration contributes significantly to the evaluation of these quantities. This makes it very difficult to solve critical phenomena using an analytical method such as perturbation theory. In other words, the system has too many degrees of freedom to solve it exactly. One breakthrough to overcome this difficulty is the so called renormalization group (RG) technique. The basic idea of RG is that near the critical point the correlation length diverges and the long distance properties of the system are not affected by details at the microscopic level. So the details of the microscopic level can be integrated out, yielding the reduced correlation length in a new lattice unit. This procedure may be called blocking of the lattice. By this procedure, it is obvious that the number of degrees of freedom of the system is reduced. Furthermore, the momentum cut-off of the system is also reduced, which implies that the coupling constants should be renormalized. Critical exponents are derived from analyzing how the couplings change under this blocking procedure. The problem of the RG is that the handling of errors due to blocking is hardly rigorous in most cases.

At values of β different from the critical β (denoted by β_c) the system is not infinitely correlated, meaning that $G(x_1, x_2)$ decays exponentially. At β_c the system is infinitely correlated, meaning that $G(x_1, x_2)$ decays much more weakly than the exponential decay. To be more specific,

$$G(0, x) \propto e^{-x/\xi} \quad \text{if } \beta \neq \beta_c \tag{1.27}$$

and

$$G(0,x) \propto \frac{1}{x^{d-2+\eta}} \quad \text{if } \beta = \beta_c \tag{1.28}$$

By Fourier transforming both sides of the eq.(1.27)

$$l.h.s = \int dx\ e^{ipx} G(0,x) = \tilde{G}(p) \tag{1.29}$$

$$r.h.s = \int dx\ e^{-x/\xi} e^{ipx} \propto \frac{1}{p^2 + (1/\xi)^2}, \tag{1.30}$$

from which

$$\tilde{G}(p) = \frac{C}{p^2 + (1/\xi)^2}, \tag{1.31}$$

where C is the proportionality constant in eq(1.30). Noting that the renormalized mass is defined as the pole of the Fourier conjugate of the two point Green's function, one can immediately conclude that the renormalized mass m_R is

$$m_R = \frac{1}{\xi}. \tag{1.32}$$

In the finite system with the linear extension L the linear momentum is quantized,

$$p_i = 2\sin(\pi n_i/L), \tag{1.33}$$

where p_i is the i-th component of $\vec{p}$ and n_i is a non-negative integer. Removing the constant C in eq(1.31) we obtain

$$\xi = \frac{1}{2\sin(\pi/L)} \sqrt{(\tilde{G}(0) - \tilde{G}(2\sin(\pi/L)))/\tilde{G}(2\sin(\pi/L))}. \tag{1.34}$$

Near the critical point where the correlation length is still finite but large enough, various physical quantities scale according to certain scaling functions. At β_c it is evident that the two point Green's function has scale invariance. Solving the Callan Symmanzik equation[2] in the deep Euclideen region is known to have a certain scale invariance also. Deep Euclidean region refers to the region where the mass of the physical system is negligible, and without a mass term any theory without a momentum cutoff displays scale invariance. Note that approaching the critical point means the mass of the system vanishes. Besides certain exceptions

such as the Kosterlitz-Thouless[3] phase transition, it is generally believed that any thermodynamic quantity X scales according to the scaling form

$$X = A|\beta - \beta_c \ |^{\rho}| \ln B|\beta - \beta_c \ ||^{\tilde{\rho}} + C. \tag{1.35}$$

Here A,B and C are constants, and ρ and $\tilde{\rho}$ are the critical exponents for power and logarithmic scaling respectively. The correction terms to the leading power scaling are called confluent terms. In the discussion of the 3D Ising model the nonanalytic confluent term will be discussed further. For χ, ξ and C_v the corresponding critical exponents are γ, ν and α respectively. Thanks to the exact solution of free energy of the 2D Ising model [4], the values of γ,$\tilde{\gamma}$, ν, $\tilde{\nu}$, α and $\tilde{\alpha}$ are known to be $4/7, 0, 1, 0, 0$ and 1 respectively. For the 4D Ising model, there is general agreement that the scaling behavior of χ, ξ and C_v is that of the mean field theory of the Ising model with the multiplicative logarithmic correction. This belief is supported by the renormalization group equation arguments[5], and was rigorously proved by Hara et al [6]. Therefore, for the 4D Ising model the values of γ, $\tilde{\gamma}$, ν, $\tilde{\nu}$ and α are 1, 1/3, 1/2, 1/6 and 0 respectively.

For the 3D Ising model, it is generally believed that the scaling form does not include the logarithmic confluent terms. However, recently the scaling form with an additive nonanalytic term

$$X = At^{\rho}\{1 + c_{\theta}t^{\theta} + c_1 t + \cdots\} \tag{1.36}$$

has been advocated by certain series expansion experts [7]. It is generally believed that with the inclusion of this term the critical exponents satisfy the hyperscaling relation

$$\Delta = \frac{1}{2}(D\nu + \gamma), \tag{1.37}$$

where Δ defined later. For a detailed discussion, we will come back to this point later, in chapter five of this dissertation.

For the definition of the renormalized 3-point coupling constant(g_R^3) and

the renormalized 4 point coupling constant(g_R^4), note that all the connected n-point Green's functions $G(x_1, \ldots, x_n)$ (n=3,4,...) vanish identically for the non-interacting theory. Therefore g_R^3 and g_R^4 at zero momentum can be defined as follows.

$$g_R^3 = -\sum_{x_1,x_2,x_3} \frac{G(x_1,\ldots,x_3)}{\chi^{2/3}}(L/\xi_L)^{D/2} \tag{1.38}$$

$$g_R^4 = -\sum_{x_1,x_2,x_3,x_4} \frac{G(x_1,\ldots,x_4)}{\chi^2}(L/\xi_L)^{D}. \tag{1.39}$$

Note that both g_R^3 and g_R^4 are wave function renormalization independent. They are defined at zero total momentum because of the sum over coordinates. Note that in the symmetric phase g_R^3 vanishes identically. From this, and using the translation invariance,

$$g_R^4 = \left(3 - \frac{< S^4 >}{< S^2 >^2}\right)(L/\xi_L)^D \tag{1.40}$$

where S is the sum of all spins over the whole lattice.

Binder's cumulant U_L on a lattice with linear extension L is defined as

$$U_L = \left(3 - \frac{< S^4 >}{< S^2 >^2}\right). \tag{1.41}$$

This quantity plays a very important role in analyzing the finite size scaling, which will be discussed in more detail in chapter three. We define

$$U_4(x_1,\ldots,x_4) \equiv < \sigma_{x_1} \cdots \sigma_{x_4} >_c \tag{1.42}$$

and

$$|\bar{U}_4| \equiv \sum_{x_2,x_3,x_4} |U_4(0,x_2,x_3,x_4)|. \tag{1.43}$$

From these definitions, it is straightforward that in the symmetric phase

$$g_R^4 = |\bar{U}_4|/(\chi^2\xi^D). \tag{1.44}$$

The critical exponent Δ is defined from the scaling behavior of $|\bar{U}_4|$. Namely, with the definition of $t = (\beta_c - \beta)/\beta_c$,

$$|\bar{U}_4| \propto t^{-(\gamma+2\Delta)}. \tag{1.45}$$

1.3 High Temperature Expansion and its Application to The Critical Phenomena

Analyzing the high temperature or the low temperature expansion of a certain statistical model whose rigorous solution is not known has been a very powerful method to estimate β_c and various critical exponents. Moreover, new techniques for overcoming such problems as the explicit inclusion of confluent singularities into methods of series analysis have been developed[7]. Among these various techniques, we will describe only two methods which are adequate in relation with the arguments of the α value of the 3D Ising model. For details, consult Guttmann[7](See also chapter five of this dissertation).

Consider the partition function

$$Z(\beta) = \sum_{\sigma_N=\pm 1} \cdots \sum_{\sigma_1=\pm 1} \exp\{\beta \sum_{<i,j>} \sigma_i \sigma_j\}. \tag{1.46}$$

If β is sufficiently small, Z(β) can be expanded in a power series of β. First, observe that for the Ising variable σ,

$$\exp(\beta\sigma) = \cosh\beta + \sigma \sinh\beta. \tag{1.47}$$

Applying this to eq.(1.46) yields,

$$\begin{aligned} Z(\beta) &= \sum_{\sigma_N=\pm 1} \cdots \sum_{\sigma_1=\pm 1} \prod_{<i,j>} (\cosh\beta + \sigma_i\sigma_j \sinh\beta) && (1.48) \\ &= (\cosh\beta)^{2N} \sum_{\sigma_N} \cdots \sum_{\sigma_1} \prod_{<i,j>} (1 + \sigma_i\sigma_j \tanh\beta). && (1.49) \end{aligned}$$

Expanding $\prod_{<i,j>} (1 + \sigma_i\sigma_j)$, it can be expressed as a sum of all the powers of *link variables* over all possible links $< i, j >$ on the lattice. *Link variable* implies the product of two Ising spins σ_i and σ_j associated with the link $< i, j >$. Since $\sum_{\sigma=\pm 1} = 0$, the sum over all the spins which are covered by odd number of links should vanish. In addition, no link can be covered more than once. So, all the contributions to the partition function come from closed link configurations, and

for each link a factor $\tanh\beta$ can be attributed. Therefore we get an expression for $Z(\beta)$:

$$Z(\beta)e^{-N}\cosh\beta^{-2N} = 1 + a_1(\tanh\beta)^4 + a_2(\tanh\beta)^6 + a_3(\tanh\beta)^8 + \cdots. \quad (1.50)$$

Here a_1, a_2 and a_3 are all the possible number of configurations which consist of four closed links, of six closed links, of eight closed links, etc respectively.

Thus, the general form of the high temperature expansion for a physical quantity X will be

$$X = \sum a_n \beta^n \quad (1.51)$$

Given the above series, a useful theorem is that if

$$a = \lim_{n\to\infty} \inf|a_{n+1}/a_n| \text{ and } A = \lim_{n\to\infty} \sup|a_{n+1}/a_n| \quad (1.52)$$

(so that $a \leq A$) the series converges for $|\beta| < A^{-1}$ and diverges for $|\beta| > a^{-1}$. In most cases, $\lim_{n\to\infty} |a_{n+1}/a_n|$ exists and is equal to either a or A, and the theorem says that the circle $\beta = a^{-1} = A^{-1}$ contains at least one point of singularity . It is worth mentioning that there may be more than one singularity on the circle.

For the study of power scaling form without any nonanalytic confluent terms, there is a widely used method of series analysis, which is primarily due to Domb and Sykes[8]. This can be proved using Darboux's theorem, which is stated in detail in the book by Guttmann[7]. According to this theorem, if a function F behaves as

$$F(z) \simeq A\left(1 - \frac{z}{z_c}\right)^{\rho} + B \quad (1.53)$$

as $z \to z_c$, then we can write

$$F(z) = \sum_{n=0}^{\infty} a_n z^n, \quad \text{where } a_n = A(z_c)\binom{n+\rho-1}{n} z_c{}^{-n}. \quad (1.54)$$

The ratio of a_n/a_{n-1} can be written as,

$$r_n = \frac{a_n}{a_{n-1}} = \frac{1}{z_c}\binom{n+\rho-1}{n}\binom{n-1}{n+\rho-2} = \frac{1}{z_c}\left(1 + \frac{\rho-1}{n}\right). \quad (1.55)$$

A plot of r_n versus $1/n$ as $n \to \infty$ yields z_c and ρ.

If A and B are entire functions, this method works rather well. Indeed, in this case one can go further and expand A(z) around z_c as

$$F(z) \sim A\left(1-\frac{z}{z_c}\right)^{\rho}\{A(z_c)+(z-z_c)A'+O(z-z_c)^2\}+B(z_c), \tag{1.56}$$

so that

$$r_n = \frac{1}{z_c}\left(1+\frac{\rho-1}{n}+\frac{c}{n^2}+O(1/n^3)\right) \tag{1.57}$$

where c can be related to A, A' and z_c .

Another ratio method which is important for this dissertation follows from Tauberian theorem, given by Feller[10][7]. If a function $G(z)$ behaves like

$$G(z) = A\left(1-\frac{z}{z_c}\right)^{-1}|\ln[k\left(1-\frac{z}{z_c}\right)]|^{\rho}, \tag{1.58}$$

where A and k are constants, one can write

$$G(z) = \sum_{n=0}^{\infty} a_n z^n \tag{1.59}$$

with

$$a_n \sim \frac{C}{{z_c}^n}[|\ln\frac{z_c}{n+1}|^{\rho}+\rho\ln\left(k\,|\ln\frac{z_c}{n+1}|^{\rho-1}\right)]. \tag{1.60}$$

Given the series(1.60) with known coefficients a_n (n=1,2,...), a least squares fit method can be applied to estimate the best values of z_c , ρ, k, and the proportionality constant. In chapter five of this thesis this fit will be done for the evaluations of the critical exponents of the 3D Ising model.

1.4 Monte Carlo Simulations

As stated before, using Feyman's path integral quantization, solving a quantum field theoretical model is formally equivalent to solving an equilibrium statistical model on a lattice. However, for a typical statistical model such as the 2D Ising

model on the lattice L=20, the total number of configurations will be 2^{400}, and averaging over all these configurations will be impossible for any available computer. Moreover, averaging over all the possible configurations is not necessary to calculate an accurate ensemble average (say within a statistical error of .1 percent).

The idea behind the Monte Carlo method is to generate a sequence of independent configurations with the probability of equilibrium distribution $exp[-\beta H(C)]$ so that for a certain thermodynamic quantity A

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} A(C_n) = \int d\mu(C) A(C) \tag{1.61}$$

$$d\mu(C) = exp[-\beta H(C)]\ /Norm, \quad \int d\mu(C) = 1.$$

The algorithms we shall consider are such that the probability of having a given configuration C_n depends only on C_{n-1} and not on the previous history of the system: sequences generated in this way are usually referred to as Markov chains. A Markov chain can be completely described by the transition probability $TP(C, C')$, which defines the probability of having $C_{n+1} = C'$ if $C_n = C$. It is obvious that for a sensible algorithm, after a finite number of operation of these transitions, any allowed C should be generated with a nonzero probability from any C'; this condition is referred as the ergodicity condition. Another condition which is a sufficient condition for a sensible algorithm is the so called detailed balance condition stated below:

$$TP(C', C) exp[-\beta H(C')] = TP(C, C') exp[-\beta H(C)]\ . \tag{1.62}$$

With these two conditions it can be easily shown that this transition probability satisfies the eq.(1.61). To be more specific, let us denote the probability for the n-th sequence to be in configuration C as $P_n(C)$. Then,

$$P_{n+1}(C') = \sum_C TP(C, C') P_n(C). \tag{1.63}$$

Summing over C in eq.(1.62) and using $\sum_C TP(C, C') = 1$, we obtain

$$P_{n+1}(C') = \exp[-\beta H(C')], \tag{1.64}$$

which shows that n+1 th configuration is generated with the desired equilibrium distribution.

Historically the first algorithm satisfying these two conditions was developed by Metropolis [11]. The updating prescription is as follows:

1. Select an arbitrary configuration C with energy $H(C)$ as starting configuration.

2. Flip spin at one or more site according to some arbitrary rule. Let the new configuration be C_T and new energy $H(C_T)$.

3. If the $H(C_T)$ has been lowered then this new configuration is accepted. If the $H(C_T)$ has been increased then the new configuration is accepted with the probability $\exp\{-\Delta H\}$, where $\Delta H = H(C_T) - H(C)$.

The problem with the Metropolis algorithm is that when the correlation length becomes considerably large the new configuration generated with this algorithm is very dependent on the initial configuration. In other words, it does not provide well distributed sampling. In order to generate an independent configuration one has to repeat this procedure a large numbers of times. (The number of sweeps to get an independent configuration from a given configuration is defined as the auto correlation time denoted by τ_{aut}.) This phenomena is the so called critical slowing down , and because of this slowing down the Metropolise algorithm becomes very inefficient for the simulations near the critical point.

To overcome this problem, a very significant breakthrough was made by Swensen and Wang (SW) [13] followed by U.Wolff [14] and A.Sokal et al [15]. To show how a cluster type algorithm can be developed, let us consider the partition function of the Ising model. Within an overall multiplicative constant,

$$Z = \sum_{\sigma_i=\pm 1} \exp \beta \sum_{<i,j>} (\sigma_i \sigma_j - 1) \tag{1.65}$$

$$= \sum_{\sigma_i=\pm 1} \prod_{<i,j>} \{(1-p) + p\delta_{\sigma_i,\sigma_j}\} \tag{1.66}$$

$$= (1-p)^{\#links} \sum_{\{\sigma_i\}} \prod_{<i,j>} \left(1 + \frac{p}{1-p}\delta_{\sigma_i,\sigma_j}\right) \tag{1.67}$$

$$= (1-p)^{\#links} \sum_{\{\sigma_i\}} \{ \prod_{<i,j>} + \prod_{<i,j>} \delta_{\sigma_i,\sigma_j}(\frac{p}{1-p})\} \tag{1.68}$$

$$= (1-p)^{\#links} \sum_{\{\sigma_i\}} \sum_{k_{ij}=0,1} (\frac{p}{1-p})^{k_{ij}} \Delta(k|\sigma). \tag{1.69}$$

Here k_{ij}'s are bond variables with values 0 and 1 and the bond probability is given by

$$p = 1 - e^{-2\beta}. \tag{1.70}$$

$\Delta(k|\sigma) \equiv \prod_{<i,j>}$ if $k_{ij} = 0$, and $\Delta(k|\sigma) \equiv \prod_{<i,j>} \delta_{\sigma_i,\sigma_j}$ if $k_{ij} = 1$. So,

$$\Delta(k|\sigma) = \prod_{ij}(\delta_{k_{ij},0} + \delta_{k_{ij},1}\delta_{\sigma_i,\sigma_j}) \tag{1.71}$$

Summing over the spins in eq.(1.69), one finds the Fortuin Kasteleyn [16] representation in terms of bonds only,

$$Z = \sum_{\{k_{ij}\}} \left(\frac{p}{1-p}\right)^{k_{ij}} 2^{n(\{k_{ij}\})}, \tag{1.72}$$

where $n(k_{ij})$ is the number of clusters for bond configuration k_{ij}, and an overall factor has been omitted.

SW's algorithm is as follows.

1. For fixed σ_i, activate k_{ij} independently link by link with probability $p \times \delta_{\sigma_i,\sigma_j}$
2. For fixed k_{ij} assign a random spin value ± 1 to each cluster as a whole.

It is clear that under this procedure large clusters of spin flip collectively, and there is a chance of improving critical slowing down. U.Wolff[14] proposed a variation of SW algorithm in the form of one cluster method. His one cluster idea is to build only one of the many SW clusters as follows:

1. Pick a random site (x_o) on the lattice.

2. Build the cluster C connected to x_o using the same bond probability as for SW.

3. Flip all spins in C.

This algorithm also satisfies both ergodicity and the detailed balance condition[14]. Moreover, several test runs have been done indicating that one cluster type algorithm has a much shorter τ_{aut} than that of SW's for some particular variables. A rigorous proof has been made by Sokal et al [17] that any kinds of multi-clusters and multigrid algorithms actually undergo the critical slowing down unless the critical exponent α of the specific heat is zero. Of course the critical slowing down of the multi-clusters and multi-grid is weaker than that of Metropolis. However they could not prove this for the one cluster type algorithm. The above facts seem to suggest that the one cluster type is more efficient than any other algorithm known so far.

Now let us sketch the general methodology and define some terminology which will be used throughout this dissertation.

1. Investigation of the finite size effects of the system with L^D:
   It is widely assumed that the effect of finite size is only dependent on the ratio $\frac{L}{\xi}$, and there exists a certain value of L (denoted by $\tilde{L}$) above which the measurements of a certain physically well defined quantity yields the thermodynamic value of that quantity. In general, the values of $\tilde{L}$ depend on the physical quantities under consideration.

2. Thermalization:
   From a given initial configuration, the system should be allowed to reach the *equilibrium configurations*. By equilibrium configurations, we mean typical configurations characteristic of the given temperature. For example, if β is

very small, then the typical configurations characteristic of that value of β will have very randomly distributed spins over the lattice. So if the initial configuration happens to be very ordered then one has to wait until the configuration becomes more disordered before starting the measurements. How many sweeps are needed to reach the equilibrium is decided by starting with two different initial configurations and by watching when the two measurements start to yield close values. This number will be denoted by NEQ.

3. Once the thermodynamic ratio and NEQ are determined, then one calculates the τ_{aut} defined before for each quantity which is supposed to be measured. Once τ_{aut} is determined the measurements of that particular quantity will be per that number of updating clusters. In practice, we binned the clusters and took the bin average and the standard deviation for that number of bins. From here on, the number of configurations over which the measurements are made will be denoted as NM and the numbers of bins will be denoted as NBIN.

To show how well the the one cluster type Monte Carlo simulation works , the data obtained for the 2D Ising model is presented in Table(1.1). For the 2D Ising model, the exact solution for the free energy in the absence of a magnetic field is known from Onsager's work[4]. The exact formula for correlation length and the value of β_C are also known, namely

$$\xi = \frac{1}{\ln \coth \beta - 2\beta} \tag{1.73}$$

$$\beta_C = \ln \sqrt{2} + 1/2 = 0.44069. \tag{1.74}$$

Here we fixed the ratio $L/\xi \simeq 6$ which is the thermodynamic ratio. For each β, there are four different bins each of which consists of 100,000 $\times$ 15 clusters. Among them 100,000 measurements were made per every 15 clusters.

In order to see how accurate the data is, let us compare our data for ξ with the exact values of ξ at the points of β, which are 4.748, 5.932, 6.824, 7.966,

9.553, 11.906 and 15.758 respectively up to order of 10^{-3}. As seen in table (1.1), the data obtained here fits the exact values within the statistical error. Our data of g_R^4 is consistent with the rigorously proven fact that a nontrivial continuum limit for the 2D Ising model exists. In order to see the consistency of our χ and C_V, we must perform a fit.

The basic idea of fitting is the same for the linear fit and the nonlinear fit. And for many cases, the non-linear fitting can be modified to be suitable to the linear fit. The idea of linear fitting is to fit N numbers of data, say $(x_1, y_1), \ldots, (x_N, y_N)$, to the function

$$y = \sum_{j=1}^{M} a_j f_j(x). \tag{1.75}$$

Here, the function forms of $f_i(x)$ $(i = 1, 2, \ldots, M)$ are known; the unknowns are coefficients a_i $(i = 1, 2, \ldots, M)$. Note that the coefficients are completely linear. Now let us define χ^2 as

$$\chi^2 = \sum_{i}^{N} \frac{1}{{\sigma_i}^2} (\sum_{j=1}^{M} a_j f_j(x) - y_i)^2. \tag{1.76}$$

Here it is assumed that the data for y_i have Gaussian distribution with the standard deviation σ_i. Obviously, the best fit will be at the point where χ^2 is minimized. So, it is trivial to solve for the minimum of χ^2 for the linear fit by solving the linear equation,

$$\frac{\partial \chi^2}{\partial a_k} = 0. \tag{1.77}$$

By defining a matrix α_{kj} and a vector β_k by

$$\alpha_{kj} = \sum_{i=1}^{M} \frac{f_k(x_i) f_j(x_i)}{{\sigma_i}^2} \tag{1.78}$$

$$\beta_k = \sum_{i=1}^{M} \frac{f_k(x_i) y_i}{{\sigma_i}^2}, \tag{1.79}$$

the eq.(1.77) reduces to the matrix equation

$$\sum_{j=1}^{M} \alpha_{kj} a_j = \beta_k, \tag{1.80}$$

and this form of equation can be easily solved by certain computer programs. To calculate the error in the estimation of a_j's note that

$$\sigma^2(a_j) = \sum_{j=1}^{N} {\sigma_i}^2 \left(\frac{\partial a_j}{\partial y_i}\right)^2. \tag{1.81}$$

Note that α_{kj} is independent of y_i , so that

$$\frac{\partial a_j}{\partial y_i} = \sum_{k=1}^{M} C_{jk} f_k(x_i)/{\sigma_i}^2, \tag{1.82}$$

where C_{jk} is the inverse matrix element of α_{jk}. From these two relations, it is trivial to show that

$$\sigma^2(a_j) = C_{jj}. \tag{1.83}$$

Finally, the goodness-of-fit of data to the model must be estimated. Without this estimation, we have no indication that the parameters obtained above have any meaning at all. This can be done by evaluating the incomplete gamma function,

$$Q(a,x) \equiv \frac{\Gamma(a,x)}{\Gamma(a)} \equiv \frac{1}{\Gamma(a)} \int_x^\infty e^{-t} t^{a-1} dt (a > 0). \tag{1.84}$$

It has the limiting value

$$Q(a,0) = 1 \quad \text{and} \quad Q(a,\infty) = 0, \tag{1.85}$$

and is monotonically decreasing with respect to x. In *numerical recipes* [18] $GAMMQ(a,x)$ is the program for the evaluation of $Q(a,x)$. Now we define the number of degree of freedom Ω by

$$\Omega = \text{thenumberofdata}(N) - \text{thenumberofparameterstofit}(M). \tag{1.86}$$

Then Q is defined as

$$Q = Q(\Omega/2, \chi^2/2), \tag{1.87}$$

which gives a quantitative measure for the goodness-of-fit of the model. If Q is very small for a particular set of data then the possibility is that at least one of the following is true;

1. The model is wrong.

2. The σ_i are really larger than stated.

3. The measurements errors are not normally distributed.

On the other hand if Q turns out to be too close to 1, then the diagnosis for this can be either the errors are overestimated than they are or the data are *fudged* to fit the model.

As stated in the previous section, as $\beta \rightarrow \beta_c$, the physical quantity X behaves asymptotically as

$$X = A(\beta_c - \beta)^{-\rho}, \quad \beta < \beta_c \ . \tag{1.88}$$

From now on, we will call this type of scaling the standard fit. However, á priori it is not known from what value of β the standard fit yields *good* results. In order to answer this question, we tried to fit the exact data of correlation length at the range of β given in Table(1.1) to the standard fit. By good is meant that the deviations are less than 10^{-3} so that the error of each point is 5×10^{-4}. Note that the data are not normally distributed, so that the value of χ^2 itself does not have any meaning in this case. As the result it gives $\beta_c = .44125(10)$ and $\nu = 1.04348(1)$. To improve the estimation of β_c and other critical exponents in the standard fit one has to go deeper inside the scaling region.

An improved form of the standard fit is

$$X = A(\beta_c - \beta)^{-\rho}\{1 + B(\beta_c - \beta)\}. \tag{1.89}$$

The same data fitting to eq(1.89) gives $\beta_c = .44066(1)$ and $\nu = .99717(1)$, which shows a surprising agreement with the true value. From these two examples it is obvious that the improved scaling form eq(1.89) yields a better estimate of β_c and critical exponents. Let us continue this test for χ also. Trying to fit the data in Table(1.1) to the standard fit yields $\beta_c = .4404(5)$ and $\gamma = 1.737(18)$. However

Table 1.1: A Monte Carlo run for the 2D Ising Model based on the single cluster algorithm

β	L	χ	ξ	g_R^4	C_V
.39	30	42.58(.07)	4.747(.016)	14.4(.2)	0.3815(.0011)
.40	36	62.54(.43)	5.962(.036)	14.2(.3)	0.4358(.0023)
.405	40	78.17(.06)	6.787(.033)	14.3(.2)	0.4697(.0017)
.41	48	102.27(.58)	7.992(.041)	14.3(.2)	0.5062(.0011)
.415	58	139.12(.49)	9.499(.037)	14.4(.3)	0.5481(.0055)
.42	72	201.83(.96)	11.778(.038)	14.1(.4)	0.6071(.0053)
.425	100	330.06(1.92)	15.724(.073)	14.4(.4)	0.6759(.0107)

the improved form of fit eq.(1.89) yields $\beta_c = .4408$ and $\gamma = 1.789(3)$. The latter result does not mean that, for the case of χ, the improved fit does not yield better estimate of β_c and critical exponents, but it does mean that in order for the improved fit to be effective very good data is needed. Without this, the fit tends to be unstable and it is possible to get into false minima. It seems that, in general, the result of fit of χ gives a better estimate than that of correlation length within a same range of the correlation length. Finally, by fixing β_c at the exact value the standard fit gives $\gamma = 1.743(6)$.

CHAPTER 2

TRIVIALITY PROBLEMS IN QUANTUM FIELD THEORY

2.1 A Brief History of Triviality Problems

Historically the triviality problem was first suggested by Landau and co-workers [19], who summed the loop diagrams for the photon propagator $D^{\mu\nu}(p^2)$ of QED in the limit of large momentum transfer p^2. Using the perturbation theory with the Landau gauge they obtained

$$\alpha_R D^{\mu\nu}(p) = -\frac{1}{p^2}(g^{\mu\nu} - p_\mu p_\nu) d(p^2, \alpha_R). \tag{2.90}$$

In this limit $d(p^2, \alpha_R)$ has a power series expansion,

$$d(p^2, \alpha_R) = \alpha_R \left(1 + \tfrac{\alpha_R(t)}{3\pi} + (\tfrac{\alpha_R(t)}{3\pi})^2 + \cdots\right) = \frac{\alpha_R}{1 - \frac{\alpha_R(t)}{3\pi}} \tag{2.91}$$

with, $t \equiv ln(p^2/m^2)$. From eq.(2.90) and eq.(2.91), it is evident that for some finite p^2, having the value of $m^2 exp(3\pi/\alpha_R)$, the propagator cannot be defined. This pole is the so called Landau ghost, and the existence of this pole means that if the perturbative feature is correct even in the nonperturbative regions, the theory cannot be defined without a certain momentum cutoff which prohibits the existence of this pole. If one wants full considerations of momentum transfer p^2, the only way to make sense of eq.(2.90) is $\alpha_R = 0$. So the theory becomes noninteracting (trivial) with the removal of momentum cutoff. With the definition of β function, it is straightforward to show that any theory with the perturbative β function,

$$\beta(g_R) = C g_R^2 \tag{2.92}$$

with positive valued constant C, leads to the running coupling constant

$$g_R(t) = \frac{g_R(0)}{1 - C\ g_R(0)t}, \tag{2.93}$$

so the problem of *ghost* has again manifested itself.

For ϕ^4 theory, the perturbative β function to the lowest order can be easily calculated as

$$\beta(g_R\ ) = \frac{3}{32\pi^2} g_R\ ^2. \tag{2.94}$$

So it would be very natural to expect the same behavior as QED. Regarding the triviality of ϕ^4 , it was K.Wilson[20] who, after his renormalization group equation calculations, suggested that ϕ^4 theory is also trivial in dimension 4.

2.2 The Continuum Limits of the Ising Model

The triviality of quantum field theories in four dimensions (4D) which are not asymptotically free in perturbation theory has been advocated for many years now. Both theoretical and numerical studies have been concentrated on the $\lambda\phi^4$ model, relevant to the Weinberg-Salam model. Not only is there general agreement that the model becomes a free field theory in the continuum limit, but several groups have translated that information into upper bounds on the mass of the Higgs particle [21]. A different point of view has been expressed by Branchina et al [22], who contend that in the phase with spontaneous symmetry breaking, a nontrivial continuum limit exists. In this dissertation we will present the results of what we believe are the most extensive numerical studies regarding the continuum limit of the Ising model in 2D,3D and 4D; they indicate that whereas several nontrivial limits can be constructed for $D < 4$, all continuum limits in 4D are trivial.

Let us briefly review the issue of triviality. In the Feynman path integral approach to quantization, the functional integral is undefined without introducing space-time discretization (except for the Gaussian case). Consequently for the

$\lambda\phi^4$ model, the functional integral is defined via the following expression:

$$Z = \left(\prod_{i\in\Lambda}\int_{-\infty}^{\infty} d\phi_i\right)\exp\{-\sum a^D[\frac{1}{2}z\left(\frac{\phi_i-\phi_j}{a}\right)^2 + \frac{m^2}{2}z{\phi_i}^2 + \frac{\lambda}{4}z^2{\phi_i}^4]\} \quad (2.95)$$

Here $\Lambda \subset \mathbf{Z}^D$, a is the lattice spacing, m and λ are the bare parameters and z is the wave function renormalization. In the usual parlance of particle physics, the continuum limit is achieved by letting $a \to 0$, while adjusting suitably the bare parameters m and λ and the wave function renormalization constant z in such a way that the Green's functions of ϕ_x approach well defined limits. The lattice spacing a is not a dimensionless quantity, hence a better specification of the limit $a \to 0$ is needed. It comes from observing that eq.(2.95) can also be regarded as the partition function of a certain lattice model. This model depends upon two parameters - the others can be scaled out. In general its truncated correlation functions decay exponentially at large (lattice) distances. However for suitably chosen values of the two relevant parameters, the correlation length may become infinite. This situation could be regarded as having let the lattice spacing go to zero, since the correlation length describes the physically meaningful distances. Therefore constructing the continuum limit of a quantum field theory is equivalent to studying the critical behaviour of a certain statistical mechanics model. We are emphasizing this point because most papers on the subject refer to the continuum limit as $a \to 0$ and in fact a can obviously be scaled away, so it should be regarded as 1.

To complete this brief review of the triviality problem, let us assume first that the parameters in eq(1) are such that $<\phi>=0$ and the correlation length is finite. We are interested in the behaviour of the Green's functions of the lattice model at distances which are asymptotic in lattice units, yet finite in physical units. The central limit theorem guarantees that at such distances the 2n-point ($n \geq 2$) Green's function becomes a sum of products of 2-point functions. Consequently, the renormalization group invariant introduced by Binder [12]

$$U_L(\{\phi\}) = 3 - \frac{\sum_{i_1,i_2,i_3,i_4} <\phi_{i_1}\phi_{i_2}\phi_{i_3}\phi_{i_4}>}{\sum_{i_1,i_2,i_3,i_4} <\phi_{i_1}\phi_{i_2}><\phi_{i_3}\phi_{i_4}>}, \quad (2.96)$$

must vanish as $\frac{1}{L^D}$ (L-linear size of the lattice) as long as the correlation length ξ_L is finite and $< \phi >=0$. Dimensional analysis then suggests that a renormalization group invariant which does measure the non-Gaussian character of the continuum limit is

$$g_R^4 = \lim_{L\to\infty} U_L(\{\phi\})(L/\xi_L)^D \tag{2.97}$$

The quantity g_R^4 plays the role of a renormalized coupling constant at zero momentum and describes the non-Gaussian character of the symmetric, massive phase. Namely if, as one adjusts m and λ to approach some critical point, g_R^4 approaches a nonzero value, then a nontrivial massive, symmetric continuum limit exists (according to Newman's theorem[23], the larger point Green's functions are also non-Gaussian.)

Two other continuum limits could be constructed. One could approach the critical point from the phase in which $< \phi >$ is nonzero. For that purpose it is convenient to define shifted fields

$$\tilde{\phi}_i = \phi_i - < \phi > \tag{2.98}$$

Again the central limit theorem guarantees that $U_L(\{\tilde{\phi}\})$ vanishes and that

$$\tilde{g}_R^4 = \lim_{L\to\infty} U_L(\{\tilde{\phi}\})(L/\xi_L)^D \tag{2.99}$$

exists. The question of triviality concerns the limiting value of $\tilde{g}_R^4$ as the bare parameters are adjusted to reach a critical point from the phase exhibiting symmetry breaking. In such a phase though, one is not restricted to investigate 2n-point couplings and an equally good indicator of triviality is provided by the 3-point coupling

$$\tilde{g}_R^3 = \frac{\sum_{i_1,i_2,i_3} < \tilde{\phi}_{i_1}\tilde{\phi}_{i_2}\tilde{\phi}_{i_3} >_C}{\sum_{i_1,i_2} < \tilde{\phi}_{i_1}\tilde{\phi}_{i_2} >^{3/2}}(L/\xi_L)^{D/2}, \tag{2.100}$$

which should tend to a nonzero value as the critical point is approached, if the continuum limit is nontrivial.

Finally, one can attempt to construct a massless continuum limit by adjusting the bare parameters to some critical value and studying the limiting value of g_R^4 and $U_L(\{\phi\})$ as $L \to \infty$ (see below).

In this dissertation we report numerical results on the quantities discussed above. However, for computational reasons, we investigated only the Ising model, which can be regarded as a certain limiting value of the model defined in eq(1). Therefore, we studied only the approach to one particular critical point on the critical line of the lattice $\lambda\phi^4$ model. It is generally believed that all critical points on that line have identical continuum properties, however this fact remains unproven.

Before presenting our results, we would like to recall what is rigorously known about the problems we are addressing:

1. Aizenman [24] proved that for the 2D Ising model, $g_R^4 \neq 0$
2. Aizenman [24] and Fröhlich [25] separately proved that g_R^4 =0 for $D > 4$.
3. Aizenman and Graham [26] proved that in 4D g_R^4 =0 if there are logarithmic corrections to the mean field divergence of the susceptibility. This fact was established by Hara and Tasaki [6] for λ sufficiently small.
4. Gawedzki and Kupianen [27] proved that the massless continuum limit in 4D is trivial for λ sufficiently small.
5. A nontrivial continuum limit in 2D and 3D has been constructed [28] but not for the Ising model (strong coupling), the case investigated here.

The numerical study consisted in using the Monte Carlo procedure to compute normalized expectation values. We used the Wolff [14] version of the Swendsen-Wang [13] cluster method. The number of measurements depended on D and L. As an example, for tl e case of 4D, $\beta = .1490$ and L=30, We have 5 different

bins each of which consisted of 4,500,000 clusters. For thermalization, 100,000 clusters were generated for each bin.

We employed always periodic boundary conditions. Consequently, at low temperature, the magnetization was defined as the time average value of the absolute magnitude of the lattice spin. This procedure produces the correct magnetization provided a sufficiently large lattice is used. We defined the correlation length ξ_L as

$$\xi_L = \frac{1}{2\sin(\pi/L)}\sqrt{\frac{\chi}{\chi_1} - 1} \tag{2.101}$$

where

$$\begin{aligned} \chi &= \sum_{\vec{x}\in\Lambda} < \tilde{\phi}_0 \tilde{\phi}_{\vec{x}} >_C \\ \chi_1 &= \sum_{\vec{x}\in\Lambda} < \tilde{\phi}_0 \tilde{\phi}_{\vec{x}} >_C \; e^{i\frac{2\pi}{L}x_1} \end{aligned}$$

Here x_1 is denoted as the first component of $\vec{x}$.

We define the massless regime as the regime in which $\xi_\infty/L >> 1, \xi_\infty >> 1$ with ξ_L still defined by eq.(2.101). Obviously, at β_c ξ_L does not represent a true correlation length; moreover the limit $L \to \infty$ does not exist(ξ_L increases with L). For this massless regime, we continued to monitor g_R^4 as the renormalized coupling. It is only this latter function which vanishes in 4D. On the contrary, Binder's function U_L seems to converge to nonzero values in all D, in agreement with certain theoretical predictions [29]. Therefore, Binder's function U_L seems to be a good indicator for signaling critical behaviour but not triviality. (Theoretically one could modify the definition of Binder's U_L so that it can be used as an indicator of the triviality of a massless limit: namely let $\beta = \beta_c$ and consider an infinite lattice, partitioned into blocks of size L. Let $\tilde{U}_L$ be the spatial average of Binder's function defined for these blocks. Then in 4D this $\tilde{U}_L$ will vanish as L goes to ∞, indicating the Gaussian nature of the massless continuum limit [30].)

Our numerical findings are reco.ded in Tables (2.2),(2.3) and (2.4). The

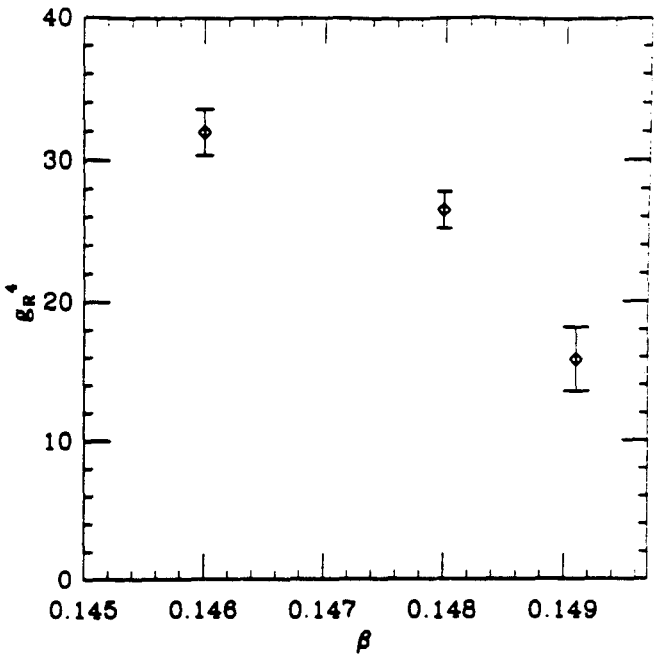

Figure 2.1: The behavior of g_R^4 in the symmetric phase of the 4D Ising model.

figure 2.1,2.2 and 2.3 illustrate the the behavior of g_R^4 , of $\tilde{g}_R^3$ and of $\tilde{g}_R^4$ in 4D respectively.

The difference between the scaling behavior of the Ising model in the superrenormalizable cases 2D and 3D and the renormalizable case 4D leaves little doubt to its trivial continuum limit in 4D. The data also suggests that taking different values of L/ξ_L does not affect these conclusions. Also, we note that there is a sign change in the four point renormalized coupling in the phase with symmetry breaking. The physical meaning of this is unclear, however we have verified the correctness of this fact through the low temperature expansion. Of course, our data covering only one point of the critical line of the $\lambda\phi^4$ lattice model, do not rule out the conjecture by Branchina et al [22] but make it unlikely. On the contrary, the data confirm nontriviality in $D < 4$ and triviality in D=4 in every phase of the Ising model.

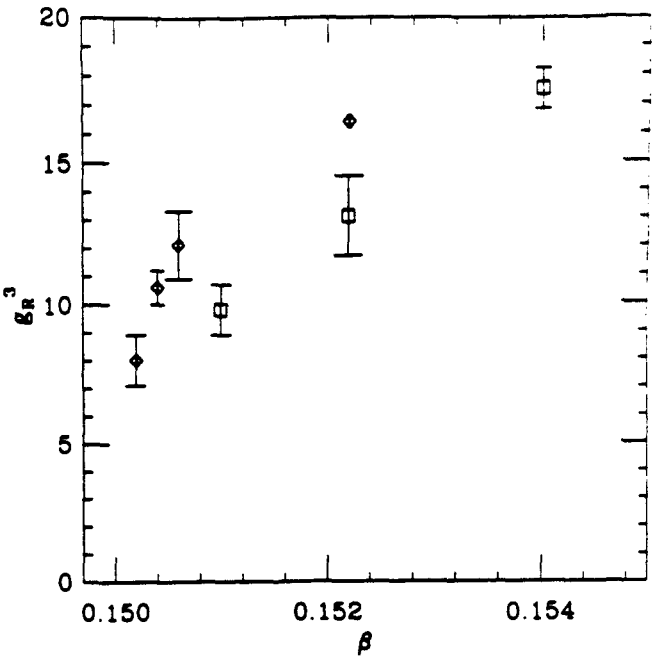

Figure 2.2: The behavior of $\tilde{g}_R^3$ in the symmetry-broken phase of the 4D Ising model.

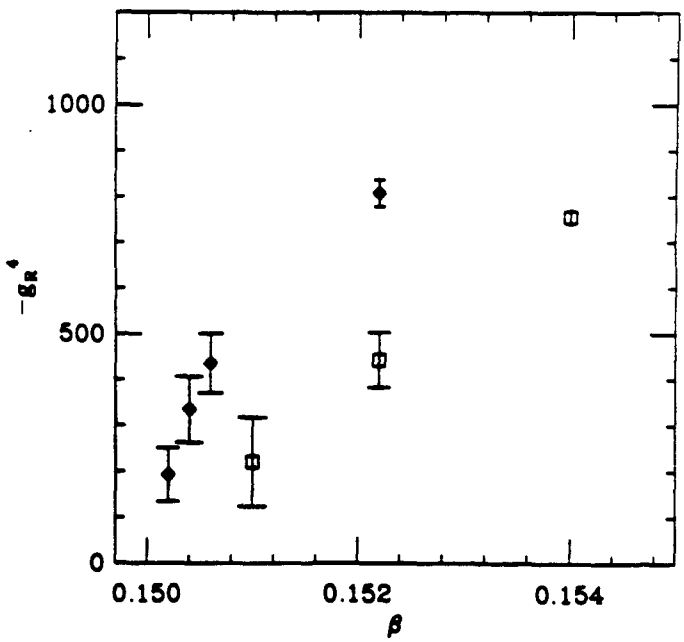

Figure 2.3: The behavior of $\tilde{g}_R^4$ in the symmetry-broken phase of the 4D Ising model.

Table 2.2: ξ_L and g_R^4 in dimensions 2, 3 and 4 in the symmetric phase. In 2D, we took two different values of L/ξ_L. $L/\xi_L \simeq 6$ is the limit above which the thermodynamic limit is reached. The data in 4D shows g_R^4 drop rapidly as β_c is approached. The supposed β_c is 0.1497.

D	β	ξ_L	L/ξ_L	g_R^4
	.40	5.96(.13)	6.04(.13)	14.0(1.1)
	.41	8.02(.26)	5.99(.19)	14.2(1.4)
	.42	11.74(.38)	6.13(.20)	14.6(1.8)
2	.425	15.76(.39)	6.03(.15)	14.2(1.9)
	.40	5.93(.09)	4.05(.6)	12.3(.4)
	.41	7.83(.09)	4.09(.5)	12.3(.4)
	.42	11.63(.16)	4.13(.6)	12.5(.6)
	.425	15.44(.19)	4.08(.5)	12.3(.6)
	.215	4.45(.02)	6.06(.03)	26.4(1.1)
	.217	5.59(.03)	6.08(.04)	26.4(1.4)
3	.220	10.89(.06)	6.06(.04)	25.1(3.3)
	.2203	12.39(.02)	6.05(.01)	26.2(3.4)
	.2206	14.53(.05)	5.99(.03)	24.1(2.0)
	.1460	3.02(.02)	3.97(.03)	32.0(1.6)
	.1480	4.65(.06)	3.88(.05)	26.5(1.3)
4	.1490	7.55(.02)	3.97(.02)	22.2(.3)
	.1491	8.13(.06)	4.03(.03)	15.8(2.3)

Table 2.3: ξ_L, $\tilde{g}_R^3$ and $\tilde{g}_R^4$ in dimensions 2, 3 and 4 in the phase with symmetry breaking. In each dimension, we took two different values of L/ξ_L; we believe that at the larger value the thermodynamic limit has been reached. In 4D, both $\tilde{g}_R^3$ and $\tilde{g}_R^4$ drop considerably fast as β_c is approached. Note the sign change in $\tilde{g}_R^4$ compared to g_R^4 in the symmetric phase.

D	β	ξ	L/ξ_L	$\tilde{g}_R^3$	$-\tilde{g}_R^4$
	.459	2.88(.05)	6.60(.11)	17.1(.3)	454(19)
	.455	3.68(.07)	6.76(.13)	16.9(.4)	438(27)
2	.425	5.72(.15)	6.65 (.17)	16.8(.4)	432(26)
	.459	4.11(.13)	9.73(.04)	24.6(.5)	1352(78)
	.455	5.36(.05)	9.51(.09)	24.2(.4)	1332(67)
	.450	7.82(.10)	9.85(.10)	23.9(.2)	1349(65)
	.2260	3.22(.01)	4.70(.02)	12.9(.2)	256(14)
	.2235	5.70(.01)	4.74(.01)	13.2(.4)	286(19)
3	.2230	6.86(.05)	4.67(.04)	12.7(.3)	260(12)
	.2250	3.62(.01)	7.97(.01)	16.0(.2)	768(19)
	.2240	4.61(.06)	7.81(.2)	16.4(.5)	763(83)
	.2230	6.37(.01)	7.86(.02)	15.6(.7)	753(86)
	.1522	2.53(.04)	4.82(.07)	16.4(.2)	808(29)
	.1506	4.34(.09)	4.84(.1)	12.1(1.2)	436(65)
	.1504	4.97(.04)	4.83(.04)	10.6(.6)	335(72)
4	.1502	5.90(.08)	5.08(.07)	8.0(.9)	193(59)
	.154	1.70(.01)	7.06(.04)	17.5(.7)	756(15)
	.1522	2.39(.03)	7.11(.09)	13.1(1.4)	444(60)
	.151	3.43(.08)	7.01(.2)	9.8(.9)	221(97)

Table 2.4: ξ_L and g_R^4 in dimension 2, 3 and 4 in the massless phase

D	β	L	U_L	ξ_L	L/ξ_L	g_R^4
2	$\ln(\sqrt{2}+1)/2$	25	1.832(1)	22.66(4)	1.10(0)	2.23(1)
		75	1.832(1)	67.64(28)	1.11(1)	2.25(2)
		125	1.833(3)	113.02(54)	1.11(2)	2.24(7)
3	.22165	32	1.415(1)	20.51(3)	1.56(0)	5.37(1)
		48	1.406(1)	30.73(5)	1.56(0)	5.36(7)
		72	1.389(3)	45.69(7)	1.58(0)	5.44(3)
4	.1497	20	1.070(3)	13.98(7)	1.43(1)	4.50(5)
		30	1.069(8)	21.68(11)	1.38(1)	3.94(6)
		40	1.080(20)	29.61(28)	1.35(2)	3.66(14)

CHAPTER 3

FINITE SIZE SCALING OF THE 4D ISING MODEL

Finite size scaling(FSS), formulated for the first time in 1971 by Fisher [30] has been used in a variety of ways to extrapolate results obtained in a finite system to get information appropriate to the infinite system. FSS is especially useful near the critical point, since at this point one needs a very large lattice size to reach the thermodynamic limit. The basic assumption of FSS is that, if one measure any physical quantity on a finite lattice with the linear extension L, then the effects of finite size effect only depend on $\frac{L}{\xi_\infty}$. Namely at a temperature $t \equiv \frac{\beta-\beta_C}{\beta_C}$,

$$\frac{P_L(t)}{P_\infty(t)} = f_P\left(\frac{L}{\xi_\infty}\right) \tag{3.102}$$

where $P_\infty(t)$ is the thermodynamic limit of $P_L(t)$ and ξ_∞ is the bulk correlation length at that point. The function f_P is unique in the sense that it does not depend on the type of the lattice used; it only depends on the quantity P under consideration. From the eq.(3.102), it is evident that

$$\lim_{x\to\infty} f_P(x) = 1. \tag{3.103}$$

Let us assume that $P_\infty(t)$ has a power scaling behavior with the critical exponent ρ as $t \to 0$, namely

$$P_L(t) = P_\infty(t) f_P\left(\frac{L}{\xi_\infty}\right) \propto t^{-\rho}\tilde{f}_P(L^{\frac{1}{\nu}}\, t). \tag{3.104}$$

At the finite L, $P_L(t)$ must be finite even at $t = 0$, so the singular term $t^{-\rho}$must be cancelled from $\tilde{f}(L^{\frac{1}{\nu}}\, t)$. Now the power series expansion of $\tilde{f}(L^{\frac{1}{\nu}}\, t)$ arround zero should be in the form of

$$\tilde{f}_P(L^{\frac{1}{\nu}}\, t) = a_1(L^{\frac{1}{\nu}}\, t)^\rho + a_2(L^{\frac{1}{\nu}}\, t)^{\rho+1} + \cdots, \tag{3.105}$$

where a_1 and a_2 are constants depending on P. Now we get the FSS form

$$P_L(t) \propto L^{\frac{\beta}{\nu}} \tag{3.106}$$

as $t \to 0$ to leading order in t. Note that the fact $L < \infty$ and $\rho > 0$ are crucial to the above argument. However, it is clear that (3.106) is true even for $\rho = 0$ by noting that any quantity with $\rho = 0$ can be written as a ratio of two quantities having the same power. The famous example for this is the so called Binder's cumulant(U_L)[12]. For Ising type spins using a set of rigorous inequalities it can be shown that U_L defined by

$$U_L = \left(3 - \frac{< S^4 >}{< S^2 >^2}\right) \tag{3.107}$$

satisfies

$$0 \leq U_L \leq 2. \tag{3.108}$$

From this inequality, the finite size scaling form

$$U_L = \tilde{f}(L^{\frac{1}{\nu}}\ t) \tag{3.109}$$

follows. This states that, for $t \simeq 0$, Binder's cumulant does not depend on L unless L is so large that $L^{\frac{1}{\nu}}\ t \neq 0$. Another important property of U_L is that in the symmetric phase for sufficiently large L,

$$U_L \propto \left(\frac{1}{L}\right)^D. \tag{3.110}$$

This relation can be easily proved using Callan-Symmanzik equation which states that once the momentum cutoff(Λ) becomes large enough, the renormalized Green's function does not change with the further increment of Λ. To be more specific

$$\frac{dG_R}{d\Lambda} \simeq 0 \ \text{ for sufficiently large } \ \Lambda. \tag{3.111}$$

So the Callan-Symmanzik equation guarantees that from a certain large L (say $\tilde{L}$) g_R^4 becomes thermodynamic. Remembering the relation between U_L and g_R^4 in the symmetric phase

$$g_R^4 = U_L \left(\frac{L}{\xi}\right)^D, \tag{3.112}$$

the relation(3.110) is obvious for $L \geq \tilde{L}$. These two properties of U_L are combined to find the critical point of the model. Some direct results of the FSS are at the critical point

$$\xi \quad \propto L \tag{3.113}$$

$$\chi \quad \propto L^{\gamma/\nu}. \tag{3.114}$$

Even though it had significant successes in describing critical phenomena in various systems[63], it was showed by Brézin[33] that in 4D this basic assumption is not correct. To be more specific, he could show that for 4D, for the $O(N)$ model, in the limit $N \rightarrow \infty$

$$\xi_L(\beta_c \ ) \propto L(\ln \ L)^{\frac{1}{4}}, \tag{3.115}$$

and argued that this behavior would not be N dependent.

In this dissertation based on Monte Carlo numerical data, we propose and determine the correction to the scaling variable. Let us assume that the *generalized* FSS variable is

$$\tilde{x} \ \equiv \frac{L}{\xi_\infty}(\ln L)^\theta \tag{3.116}$$

and that the *generalized* scaling form of a certain physical quantity $P_\infty(t)$ is

$$P_\infty(t) \propto t^{-\rho} \ |\ln \ t|^{\tilde{\rho}} \tag{3.117}$$

in 4D. This follows from non-rigorous renormalization group arguments [5] and was proved rigorously for the correlation length and the magnetic susceptibility by Hara *et al* [6]. Here t is defined as $|\frac{\beta-\beta_C}{\beta_C}|$ and θ is a model dependent *universal* quantity. We denote the critical exponents of the logarithmic correction to the leading scaling term by using a *tilde*; for example,

$$\xi_\infty(t) \propto t^{-\nu} \ |\ln \ t|^{\tilde{\nu}}. \tag{3.118}$$

We assume that the finite size effect depends only on the modified scaling variable $\tilde{x}$ so that

$$\frac{P_L(t)}{P_\infty(t)} = f_P(\tilde{x} \ ), \tag{3.119}$$

where $P_L(t)$ is the value of the quantity on a finite lattice of linear extension L. By defining the rescaled FSS variable x' by

$$x' \equiv (\tilde{x})^{\frac{1}{\nu}} = t\, L^{\frac{1}{\nu}} (\ln\ L)^{\frac{\theta}{\nu}}\, |\ln\ t|^{-\frac{\tilde{\nu}}{\nu}}, \tag{3.120}$$

eq(3.119) can be written as

$$P_L(t) = t^{-\rho}\ |\ln\ t|^{\tilde{\rho}} \tilde{f}_P(x'\ ). \tag{3.121}$$

On a finite lattice there can be no singularity for any values of t, so that as $t \to 0$ the expansion of $\tilde{f}_P(x'\ )$ must be

$$\tilde{f}_P(x'\ ) \simeq a_P\ x'^{\ \rho} + b_P\ x'^{\ \rho+1} + \ldots \tag{3.122}$$

to cancel the leading singularity $t^{-\rho}$. Here a_P and b_P are constants depending only on P. To remove the logarithmic singularity the relation

$$\tilde{\rho} = \frac{\rho\tilde{\nu}}{\nu} \tag{3.123}$$

must be true. From the above relation it is evident that if the correlation length has a multiplicative confluent correction to the leading power scaling, any other quantity whose leading singularity is a power must also have a multiplicative confluent correction and vice versa. We stress that the relation(3.123) is model independent. Note also that this relation is consistent with the rigorous result [6] ($\tilde{\gamma}$=1/3 and $\tilde{\nu}$=1/6).

Finally we obtain the leading FSS form

$$P_L(0) = a_P L^{\frac{\rho}{\nu}} (\ln\ L)^{\frac{\theta\rho}{\nu}}. \tag{3.124}$$

A direct consequense of this is that

$$\xi_L(0) \ \propto\ L\ (\ln L)^{\theta} \tag{3.125}$$

$$\chi_L(0) \ \propto\ L^{\gamma/\nu} (\ln\ L)^{\gamma\theta/\nu}. \tag{3.126}$$

Here the magnetic susceptibility and correlation length on finite lattice with linear extension L are defined as

$$\chi_L = \frac{1}{|\Lambda|} < S^2 >, \; S \equiv \sum_{\vec{x}\in\Lambda} \sigma_{\vec{x}} \tag{3.127}$$

$$\xi_L = \frac{1}{2\sin(\pi/L)}\sqrt{\frac{\chi}{\chi'} - 1} \tag{3.128}$$

where

$$\chi' \equiv \sum_{\vec{x}\in\Lambda} < \sigma_0 \sigma_{\vec{x}} > e^{i\frac{2\pi}{L}x_1}. \tag{3.129}$$

Here x_1 is the first component of $\vec{x}$. Motivated by the high temperature expansion result[34] (β_c =.149709(8)), we investigated FSS behavior of the Binder's cumulant(U_L)[12] at β = .148968, at .1497 and at.148972 to determine β_c precisely. The results are summarized in Tab.(3.5). At β = .1497 a very detailed numerical study has been conducted and the results are summarized in Tab.(3.6). We conclude that the critical point is .1497(±.00002) and the FSS behavior becomes stable from L=20. These results may be compared with the FSS behavior of 2D Ising model (Tab.(3.7)). In 4D, $\xi_L(0)$ is definitely not proportional to L as it is in 2D, and $\chi_L(0)$ is not proportional to $L^{\gamma/\nu}$ as in 2D. Since the leading critical exponents are known for the 4D Ising model ($\nu = 1/2$ and $\gamma = 1$), from the FSS behavior of $\xi_L(0)$ or $\chi_L(0)$, one can easily determine the value of θ by the linear least square fit, and since these fits are linear the error estimation can be done without any ambiguity[18]. From the $\xi_L(0)$ fit we obtain θ = .238(.005) and from the $\chi_L(0)$ fit we obtain θ = .269(.003). These results are shown in figure 3.4 and figure 3.5.

Our estimate seems to show good agreement with the renormalization group prediction(θ = .25) by Brézin.

We used the one cluster type Monte Carlo algorithm devised by U.Wolff [14], and the periodic boundary condition was assumed. For the case of 4D measurements for β = .1497, for each L, we had 8 bins each of which consists of .8

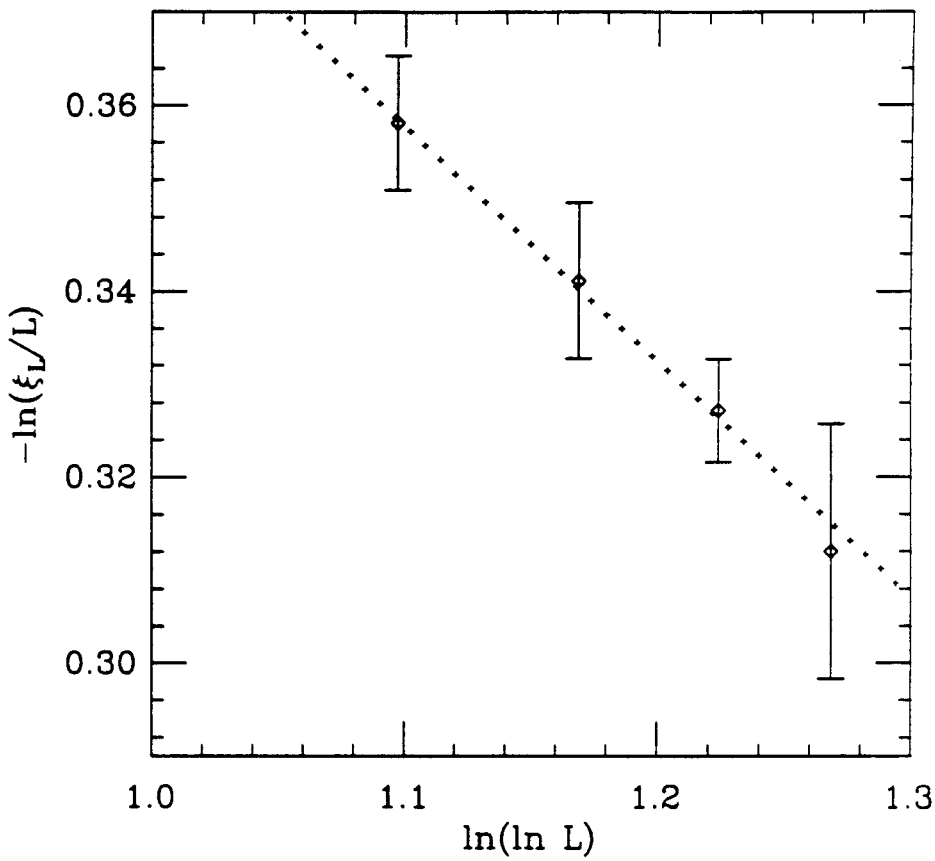

Figure 3.4: The ξ_L fit. Here diamonds represent Monte-Carlo data and dotted line represents points obtained from the fitting. The value of the slope corresponds to θ

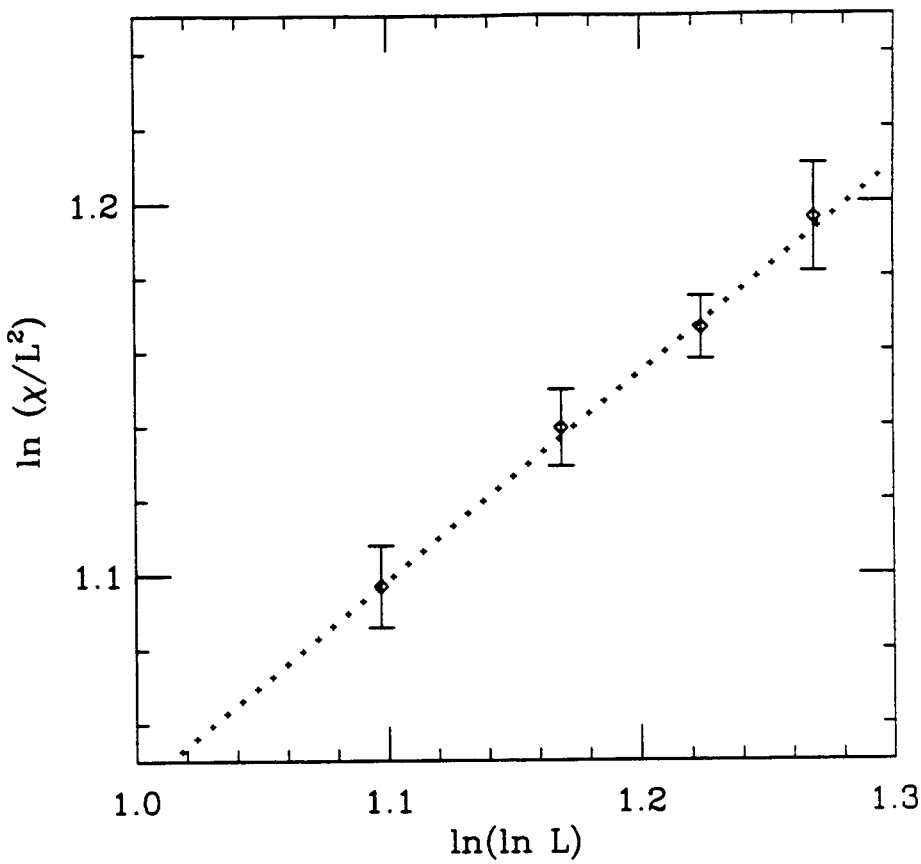

Figure 3.5: The χ_L fit. Here diamonds represent Monte-Carlo data and the dotted line represents points obtained from the fitting. The value of the slope corresponds to 2θ

Table 3.5: U_L at three different values of β. At β =.14968 U_L decreases with L, whereas at β =.14972 it increases with L. Note that U_L is almost a constant from L=20 at β =.1497

L	β = .14968	β = .1497	β = .14972
20	1.013(.002)	1.075(.019)	1.088(.002)
25	1.007(.015)	1.071(.012)	1.112(.010)
30	.953(.031)	1.056(.016)	1.123(.008)
35		1.055(.046)	1.190(.025)

million clusters. The first .1 million clusters of each bin were used for the thermalization and the averages and error estimation were obtained over these six bins.

Table 3.6: ξ_L and χ_L at β =.1497. Note that ξ_L/L and χ_L/L^2 increase uniformly as L is incremented.

L	ξ_L	ξ_L/L	χ_L	χ_L/L^2
20	13.99(.11)	.700(.006)	1201.0(13.1)	3.003(.024)
25	17.83(.07)	.713(.003)	1960.7(17.2)	3.137(.028)
30	21.63(.13)	.721(.004)	2889.0(24.5)	3.210(.027)
35	25.62(.35)	.732(.010)	4046.3(64.8)	3.303(.053)

Table 3.7: The finite size scaling study of the 2D Ising model at β = .44069. Here ξ_L/L and $\chi_L/L^{\frac{7}{4}}$ are not changed with the variation of L

L	U_L	ξ_L	ξ/L	χ_L	$\chi_L/L^{\frac{7}{4}}$
25	1.832(.001)	22.66(.04)	.906(.002)	304.8(1.7)	1.090(.006)
50	1.830(.002)	44.88(.09)	.898(.002)	1021.6(1.4)	1.087(.001)
75	1.832(.001)	67.64(.28)	.902(.004)	2083.7(2.5)	1.090(.001)
100	1.830(.006)	90.56(.24)	.906(.003)	3448.0(7.3)	1.090(.002)
125	1.833(.008)	113.02(1.94)	.904(.008)	5095.4(15.2)	1.090(.003)

CHAPTER 4

CRITICAL BEHAVIOR OF DILUTED ISING SYSTEMS

The basic idea of universality [34] is that critical behavior depends only on a small number of general features of the Hamiltonian and not on its details. For classical ferromagnets, the important features are supposed to be the dimension N of the $O(N)$ spin, the dimensionality D of the lattice, the symmetry of the interaction (in spin and real space) and its range. As an example, it is known that the nearest-neighbor (n.n.) Ising model has the same critical exponents on a square (S) or triangular (T) regular lattice. It is therefore understandable that the general consensus is that in the 2D n.n. model, critical behavior is unmodified by either bond or site dilution [35]. More specifically, suppose that for an S lattice the partition function is

$$Z\{p\} = \sum_{\sigma} \exp\{\beta \sum_{<i,j>\in \mathbf{Z}^2} p_i p_j \sigma_i \sigma_j\} \tag{4.130}$$

In eq.(1) $\sigma_i = \pm 1$ are Ising spins and the site variables p_i take preassigned values 0 or 1. If p_i=1 at all sites, the system is undiluted. The system could be site diluted in a regular or random fashion. For instance, one could prescribe that p_i=1 at certain sites forming a regular sublattice of $\mathbf{Z}^2$ and 1 otherwise. Alternatively, p_i could be treated as an independent random variable taking the value 0 (1) with probability x $(1-x)$ for some $0 \leq x$. Griffith's inequality can be used to bound from above the magnetic susceptibility of the diluted system by that of the undiluted one. Thus a high temperature phase without long range order (l.r.o.) will exists for any dilution. If the dilution is such that a percolating sublattice (of sites where $p_i = 1$) exists, then a phase with l.r.o. will also exist at sufficiently

large β.

Until 1983 it seems that the general belief was that the phase transition occuring in the diluted systems has the same critical features as in the undiluted one. Perhaps the statement is easy to accept for the case of uniform dilution, where some cases - for instance $x = 1/4$ - can be analytically related to the undiluted one: the system remains an n.n. Ising model, but β is renormalized.

The effect of random dilution is less intuitively clear and two decades ago led to some debates [35]. The simple minded picture is this: at least for x small, say 0.1 , one is making some small, randomly placed holes in the lattice. A percolating, robust, 2D lattice still exists, on which, in view of universality, one should observe the same type of critical behavior as in the undiluted model. This picture was made more quantitative by Harris and Lubenski (H-L)[36], who employed the renormalization group method of Niemeijer and van Leeuwen [37] to study critical behavior in a related *spin-glass* model. In this model, the randomness is introduced by giving each bond a random value, such that the mean is β, yet small fluctuations around the mean are allowed. On a T lattice, H-L showed that the usual Ising fixed point is stable under these type of small, random bond modifications. Of course, we were discussing a randomly diluted site model, in which the site is either occupied or not, which is a large modification, so strictly speaking the H-L result does not apply. Yet, it appears that the expectation was that the behavior of the critical site diluted model will be the same as of the undiluted one. Two Monte Carlo studies claim to have established that fact [38].

This belief was challenged in 1983 by Dotsenko and Dotsenko [39] who claimed that at least for weak bond dilution, critical behaviour does become modified, but only in a region of $O(\exp(-c/x)$ $(c > 0, x$-the weak concentration of bond impurities). This conclusion is supposed to follow from the fact that the continuum limit of the weakly diluted model is a certain 4-fermion interaction model. It leads to the surprising result that in some sense the critical diluted model is more

ordered than the undiluted one, since it has γ/ν=2 (η=0).

In this dissertation we report the results of a Monte Carlo investigation of the site diluted 2D n.n. Ising model. Our indications are that contrary to theoretical expectations and previous numerical claims, random dilution does affect critical behavior in this 2D system. We find though that the numerical study of the randomly diluted system is substantially more delicate than that of the undiluted system because of very important finite size effects.

The numerical investigation was conducted as follows: at a given value of β, we chose a square periodic lattice of size $L \times L$ and randomly diluted sites with probability x. We then conducted a Monte Carlo study of the ensuing Ising system, using the single cluster algorithm [14]. For a given random distribution of dilutions, a typical run started with 100,000 thermalization clusters; then followed measurements on 200,000 clusters separated by 20 updating clusters. The 200,000 measurements were separated into 5 bins, which allowed an estimation of the statistical error. For the magnetic susceptibility and correlation length, we estimated this error at less than 1% and 3% respectively; for the case of finite size scaling study the estimated errors are less than .5% and 1% respectively.

To monitor finite size effects, with the same L and β, we repeated the measurements on the different realizations of the random dilution process. By the ergodic theorem, in the infinite volume limit, all expectation values of translational invariant observables, such as the susceptability, become independent of the realization. Consequently at given β, one should increase L until different realizations of the dilution process produce the same results within the error of each run. It is well known that in the undiluted system the thermodynamic limit is reached for $L/\xi = 6$. To our surprise, in the randomly diluted system, even at a small dilution $x = 1/9$, reaching the thermodynamic limit requires L/ξ greater than 20. To be more specific, the error in each run is substantially smaller than the error produced by changing the realization of the diluted lattice(see Tab. (4.8) and Tab. (4.9)).

In practice, we usually generated more than 15 different realizations of random dilution at each β fixing L/ξ approximately 20, and averages were taken over the values of each realization. We define the magnetic susceptibility χ as

$$\chi = \frac{1}{|\Lambda|} < S^2 >, \; S = \sum_{\vec{x} \in \Lambda} \sigma_{\vec{x}} \tag{4.131}$$

and the correlation length ξ_L as

$$\xi_L = \frac{1}{2\sin(\pi/L)} \sqrt{\frac{\chi}{\chi_1} - 1}, \tag{4.132}$$

where

$$\chi_1 = \sum_{\vec{x} \in \Lambda} < \sigma_0 \sigma_{\vec{x}} > e^{i\frac{2\pi}{L}x_1}. \tag{4.133}$$

Here x_1 is the first component of $\vec{x}$. In Tab. (4.10) and Tab. (4.11) we give the results of our measurements for $x = 1/9$ and $x = 1/4$ respectively. Besides χ and ξ, we measured the specific heat and the four point renormalized coupling constant defined as

$$g_R^4 = U_L \left(\frac{L}{\xi_L}\right)^2 \tag{4.134}$$

$$U_L = 3 - \frac{\sum_{i_1,i_2,i_3,i_4} < \sigma_{i_1}\sigma_{i_2}\sigma_{i_3}\sigma_{i_4} >}{\sum_{i_1,i_2,i_3,i_4} < \sigma_{i_1}\sigma_{i_2} >< \sigma_{i_3}\sigma_{i_4} >} \tag{4.135}$$

The values of χ and ξ were used to determine critical exponents γ and ν. For $x = 1/9$, we obtain

$$\gamma = 2.02(\pm.13) \text{ and } \beta_c = .5385(\pm.0025) \tag{4.136}$$

from the χ fit, and fixing β_c at .5385 $\nu = 1.20(\pm.11)$ from the ξ fit. For $x = 1/4$, we obtain

$$\gamma = 2.82(\pm.45) \text{ and } \beta_c = .792(\pm.022) \tag{4.137}$$

from the χ fit, and fixing β_c at .792 $\nu = 1.73(\pm.35)$ from the ξ fit. In all cases the χ^2 per degree of freedom are between .1 and .2, and the fits (especially the χ fits) are sharp enough to see clear deviation from the undiluted system.

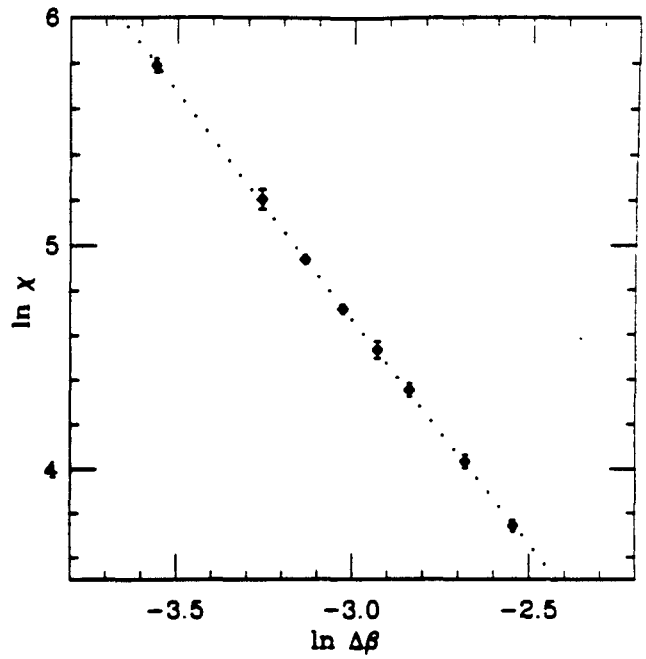

Figure 4.6: The χ fit for $x = 1/9$. The slope yields the value of γ.

To test our procedure we repeated the measurements for a lattice in which 1/9 of the sites were diluted in a regular fashion(see Tab. (4.12)). We obtain

$$\gamma = 1.748(\pm.017) \text{ and } \beta_c \quad = .5438(\pm.017) \tag{4.138}$$

from the χ fit, and fixing β_c at .5438 $\nu = 1.01(\pm.01)$ from the ξ fit.

Finally, we present the finite size scaling study results for $x = 1/9$ at β .5385 (see Tab. (4.10)).

The obtained value of γ/ν from χ_L fit is $1.77(\pm.07)$, which is consistent with our previous results from thermalization data. we believe that this is a clear indication that the value of η is not zero as claimed by Dotsenko and Dotsenko [39]. There is little doubt that our data suggest γ and ν are changed from the standard Ising values by random dilution, but not by regular dilution. Also, from ξ_L fit we obtain $\xi_L \propto L^\theta$ with $\theta = .99(\pm.13)$, which is consistent with the prediction of finite size scaling at critical point.

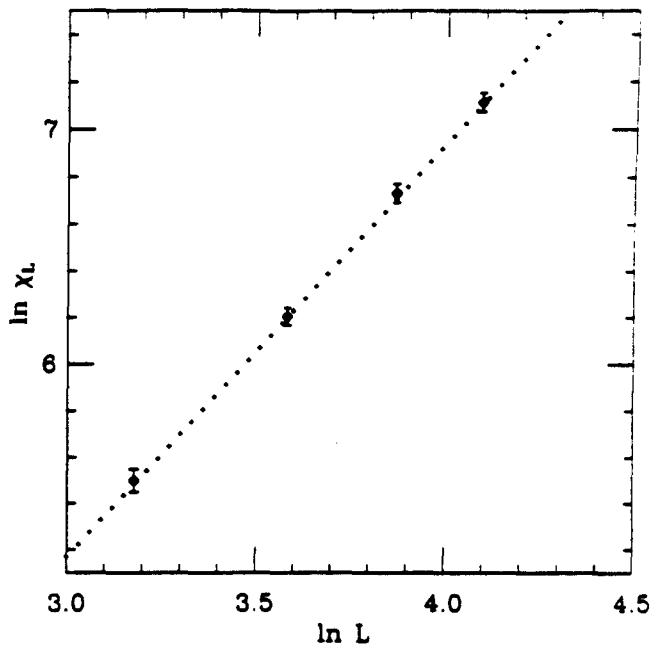

Figure 4.7: The FSS fit of χ_L for $x = 1/9$. The slope yields the value of γ/ν

Discussion:

1. That there is a dramatic difference between a regularly and a randomly diluted system can be seen from the following rigorous result, obtained by Georgii [40] (see Theorem 3.3): consider a randomly diluted S lattice and let $x < x_c$, with x_c being the critical density above which the sites where $p_i = 1$ cease percolating (for the S lattice $x_c \simeq .41$ [41]). Let i_p be any site belonging to the percolating cluster C_∞. Then there exists a $\beta_c(x)$ such that for $\beta > \beta_c(x)$ we have

$$< \sigma_{i_p} >^+ > 0, \text{ for all } i_p \in C_\infty \tag{4.139}$$

but

$$\inf_{i_p \in C_\infty} < \sigma_{i_p} >^+ = 0 \tag{4.140}$$

Obviously in a regularly diluted system, eq(4.139) would remain true, but

eq(4.140) would be false. Indeed, in a randomly diluted system, the probability to find sites connected to the percolating cluster by arbitrarily long and thin chains of occupied sites is nonvanishing. Such sites do not exist in regularly diluted systems.

2. The observation made above underlines the importance of fluctuations in understanding randomly diluted systems. Fluctuations were also at the basis of a heuristic argument advanced by Harris many years ago [43], according to which if the specific heat exponent of the undiluted system $\alpha(0) > 0$, then the randomly diluted system exhibits ordinary Ising behavior only for $|\beta - \beta_c\ (x)| > c\, x^{1/\alpha}$; for $\beta \to \beta_c\ (x)$, critical behavior is modified and for instance the specific heat does not diverge (remains $O(1/x)$). We would like to offer a modification of Harris' argument, which leads to a lower bound on the critical exponent $\nu(x)$. We already know from Georgii's result that the diluted system undergoes a phase transition. We do not know its order, but suppose it were accompanied by a divergent correlation length. In another words, assume that there exists a β_c (x) such that for $\Delta\beta \equiv \beta_c\ (x) - \beta$ sufficiently small,

$$\xi = c\Delta\beta^{-\nu(x)} \tag{4.141}$$

Now consider a region of the lattice of linear dimension ξ. The number of diluted sites in such a region is a random variable with mean $x\xi^D$ and variance $\sqrt{x(1-x)\xi^D}$. If we assume that (at least for $x < x_c$), $\beta_c\ (x)$ is a smooth function of x, we can translate the local fluctuations of x into local fluctuations of β_c. But the self consistency of the assumption that at $\beta_c\ (x)$, ξ diverges requires that

$$\xi^{-\frac{1}{\nu(x)}} > c\, \xi^{-\frac{D}{2}} \tag{4.142}$$

Therefore it must be true that

$$\frac{1}{\nu(x)} < \frac{D}{2} \tag{4.143}$$

If we further assume the hyperscaling relation

$$\alpha = 2 - \nu D \tag{4.144}$$

we conclude that

$$\alpha \leq 0. \tag{4.145}$$

Our numerical results for 2D are consistent with these conclusions.

3. Patrascioiu and Seiler [44] have proposed regarding classical $O(N)$ ferromagnets as Ising systems with random couplings. (Of course in that case, the randomness corresponds to an annealing process, while until now we have discussed only quenched dilution. However, by a novel use of ergodicity, Patrascioiu and Seiler showed how to replace the annealed process by a quenched one.) The discussion above regarding the effect of the fluctuations can be carried over and we would again expect eq(4.143) and eq(4.145). These expectations do not contradict general beliefs or numerical facts. For instance in 2D, the $O(2)$ model is expected to exhibit the Kosterlitz type of critical behavior [3], which corresponds to $\nu = \infty$. Moreover, there is general agreement that the specific heat does not diverge in any $O(N)$ model. We would guess that it is actually singular, but with $\alpha < 0$.

4. Our results contradict the H-L predictions. The morale is that the true flow of the renormalization group is more complicated than it was assumed. In the absence of estimation of the truncation error, the renormalization group arguments can lead astray (see for instance [45]).

Table 4.8: The finite size scaling study at β =.420 for $x = 1/9$. The errors denoted here and in Tab. (4.9) are solely due to different realizations of impurities. It is clear that as L increases the values of standard deviations due to different realizations of dilution decrease. However the value of standard deviation is still larger than the statistical error for a given realization.

L	χ	ξ	g_R^4	C_v
15	16.77(1.17)	2.849(.162)	17.0(1.3)	.2556(.0099)
18	17.55(1.09)	2.937(.134)	17.8(1.4)	.2522(.0075)
21	17.72(1.02)	2.967(.108)	18.1(.8)	.2514(.0059)
30	17.86(.54)	2.985(.073)	19.2(1.3)	.2499(.0045)
39	18.13(.74)	3.002(.101)	19.4(2.5)	.2507(.0049)
48	18.31(.53)	3.048(.085)	17.9(6.2)	.2517(.0037)
57	18.03(.38)	2.979(.091)	18.7(3.6)	.2495(.0033)

Table 4.9: The finite size scaling study at β =.530 for $x = 1/4$. Note that the values of standard deviation due to different realizations are generally larger than those for $x = 1/9$

L	χ	ξ	g_R^4	C_v
10	12.03(1.83)	2.607(.332)	18.1(3.8)	.2200(.0191)
20	14.50(1.85)	2.868(.255)	23.2(3.1)	.2060(.0081)
30	14.99(1.38)	2.953(.212)	25.4(4.0)	.2069(.0054)
40	14.99(1.85)	2.969(.222)	26.6(4.4)	.2056(.0070)
50	15.22(.96)	3.000(.249)	27.8(6.4)	.2054(.0046)
60	15.37(.75)	3.019(.133)	29.5(6.6)	.2079(.0026)
70	15.36(.73)	2.999(.142)	27.9(8.0)	.2068(.0036)

Table 4.10: Results for $x = 1/9$. Here NB denotes the number of different realizations at a given β. The values of g_R^4 are larger than those for the undiluted system ($g_R^4 \simeq 14.2$)

β	L	NB	χ	ξ	g_R^4	C_v
.460	102	18	42.08(1.05)	4.963(.191)	23.0(6.5)	.3330(.0047)
.470	120	23	56.43(1.61)	5.959(.278)	20.8(7.1)	.3580(.0047)
.480	141	25	77.68(2.29)	7.227(.323)	22.6(5.2)	.3822(.0034)
.485	162	14	93.00(3.42)	8.019(.397)	20.1(4.9)	.3963(.0055)
.490	180	14	111.78(2.18)	8.933(.412)	20.7(4.5)	.4099(.0053)
.495	210	12	139.71(2.64)	10.195(.412)	20.8(5.6)	.4263(.0034)
.500	240	16	182.56(8.02)	12.112(.585)	18.5(4.9)	.4429(.0060)
.510	360	18	327.62(9.60)	16.686(.765)	21.0(5.1)	.4777(.0117)

Table 4.11: The results for $x = 1/4$. From this table the values of g_R^4 obviously increase with x.

β	L	NB	χ	ξ	g_R^4	C_v
.600	100	18	36.04(1.78)	4.985(.362)	26.4(9.1)	.2429(.0029)
.620	118	17	48.38(2.29)	5.993(.237)	27.4(7.0)	.2482(.0027)
.640	148	13	71.36(4.24)	7.780(.411)	25.3(5.2)	.2545(.0050)
.660	182	15	102.66(6.56)	9.638(.584)	24.9(3.5)	.2586(.0045)
.680	240	12	163.61(9.59)	12.686(.724)	28.2(6.8)	.2600(.0037)
.700	360	15	288.30(23.60)	17.835(1.137)	26.3(6.4)	.2626(.0036)

Table 4.12: The results for $x = 1/4$. From this table the values of g_R^4 obviously increase with x.

β	L	NR	χ	ξ	g_R^4	C_v
.600	100	18	36.04(1.78)	4.985(.362)	26.4(9.1)	.2429(.0029)
.620	118	17	48.38(2.29)	5.993(.237)	27.4(7.0)	.2482(.0027)
.640	148	13	71.36(4.24)	7.780(.411)	25.3(5.2)	.2545(.0050)
.660	182	15	102.66(6.56)	9.638(.584)	24.9(3.5)	.2586(.0045)
.680	240	12	163.61(9.59)	12.686(.724)	28.2(6.8)	.2600(.0037)
.700	360	15	288.30(23.60)	17.835(1.137)	26.3(6.4)	.2626(.0036)

Table 4.13: The results for an ordered diluted system with $x = 1/9$

β	L	χ	ξ	g_R^4	C_v
.47	36	33.01(.06)	4.459(.007)	15.3(.5)	.3102(.0018)
.48	51	57.22(.03)	6.219(.019)	15.2(.6)	.3675(.0017)
.50	63	82.07(.05)	7.680(.020)	15.5(.6)	.4032(.0008)
.51	81	128.44(.50)	10.005(.033)	14.7(.3)	.4506(.0008)
.52	114	238.07(.25)	14.352(.048)	14.4(.6)	.5174(.0026)

CHAPTER 5

CRITICAL EXPONENTS OF THE 3D ISING MODEL

Probably one of the major developments in the study of the critical exponents and the critical temperature for the 3D Ising model is the introduction of the non-analytic confluent term to the usual scaling form. To be more specific, taking the example of magnetic susceptibility, the scaling form

$$\chi \sim (\beta_c - \beta)^{-\gamma}\{1 + a_1(\beta_c - \beta) + \ldots\}, \tag{5.146}$$

is replaced with

$$\chi \sim (\beta_c - \beta)^{-\gamma}\{1 + b_1(\beta_c - \beta)^{\theta} + a_1(\beta_c - \beta) + \ldots\}. \tag{5.147}$$

Currently there exists no physical explanation for this change. Based on the renormalization group equation, the value of θ was first evaluated by Le Guillou and Zinn Justin [57] to be

$$\theta = .493 \pm .007. \tag{5.148}$$

However after the HTE analysis of χ on a FCC lattice upto the 10th order in $\tanh\beta$, Camp and Van Dyke[58] concluded that the coefficient b_1 was negligible. Assuming the absence of this term, Baker analyzed various HTE using padé and ratio methods, and evaluated that in 3D

$$2\Delta - D\nu - \gamma = -.028 \pm .003, \tag{5.149}$$

which violates that particular hyperscaling relation. The validity of this hyperscaling is related with the triviality of the continuum limit of the corresponding statistical model[59], so that the violation of that hyperscaling relation means a

a trivial continuum limit of the 3D Ising model. The observation of Camp and Van Dyke was refuted later by McKenzie who analyzed the same HTE series up to 15th order in $\tanh\beta$, and estimated

$$b_1 = -.052 \pm .002. \tag{5.150}$$

Nickel[60] showed that

$$2\Delta - D\nu - \gamma \simeq 0 \tag{5.151}$$

if the non analytic confluent term is present. After Nickel there were a couple of similar calculations on different lattices, however the conclusions were not the same in all cases (see Adler[62] for the detailed descriptions).

The evaluations of various critical exponents and β_c have been continued by various groups using various methods. Le Guillou and Zinn-Justin[?] have carried out a series analysis using the fifth order ε expansion for the critical exponents. Their estimations are $\gamma = 1.2390(25)$, $\nu = .6310$, $\beta_c = .3270$ and η=.0375(25). Series analysis for the extraction of various critical exponents and their derivatives has been improved by incorporating non-analytic confluent corrections to the leading scaling behavior, and by the use of biased inhomogeneous differential equations. Guttmann[70], using the method of integral approximants obtained β_c =.221657(7), γ=1.239(3) and ν=.632(3). Nickel and Rehr [51] analyzed the 21 terms of the high temperature series for χ and ξ on a BCC lattice to get γ=1.237(2) and ν=.6300(15). The first detailed finite size scaling study was done by Barber *et al* [54] to get $\beta_c \doteq .22165$ and γ/ν=1.98. Their results have been cast into doubt by Parisi and Rapuano [64] and by Bhanot *et al* [52]. The presumed culprit was the random number generator. Recently, Ferrenberg and Landau [55] have carried out a high resolution finite size scaling analysis using the histogram techniques of Ferrenberg and Swendsen [56] to obtain β_c =.2216595(26), $\nu = .6289(8)$ and $\gamma = 1.239(7)$. Another method for analyzing the critical behavior is to numerically determine the partition function and investigate the finite size scaling of the complex zeros closest to the real temperature axis. This was first

done by Bhanot *et al* [53] yielding the estimate $\nu = .6295(10)$. Alves *et al* [57] repeated these calculations giving ν=.6285(19). Finally, Baillie *et al* al used the Monte Carlo renormalization group (MCRG) techniques to get ν=.624(2) and η=.026(3). For a nice summary of all the above results consult the paper of Baillie *et al* al [68]. The advantage of series analysis is that there are no statistical or finite size errors. However, in general, it is impossible to determine from what point in a series expansion the series become stable. Our data is summarized in table (5.14), and the result of the fitting is summarized in table (5.15). The result of the investigation of finite size effects is summarized in table (5.16).

Regarding the value of α, all of the above methods extracted their values assuming the validity of hyperscaling

$$D\nu = 2 - \alpha \tag{5.152}$$

in the 3D Ising model. This relation is valid for the 2D Ising model and is believed to be correct in the 4D Ising model also. For the 3D case, although many *believe* its validity, there is no conclusive data[65].

Historically, it was Sykes *et al* [66] who first estimated the value of α for the 3D Ising model (3DIS) based on ratio method analysis of the high temperature expansions(HTE) of specific heat on the FCC lattice. Later their HTE of specific heat was improved up to v^{14} ($v \equiv \tanh\beta$) on the FCC lattice [66] and several different HTE on the other types of lattices were obtained. It was claimed that all of their results were consistent. However, padé analysis of these series expansions was not consistent with their results[67].

It must be emphasized that in the analysis of HTE and FSS the power scaling is preassumed, which means that á priori there is no proof for power scaling of the 3D specific heat. Moreover, all the trials to prove or to disprove this hyperscaling relation also assume the power scaling behavior of 3DSPH[65]. All the estimates of α from the methods stated above lie between .11 and .12 depending on various methods[68].

In a certain sense the power scaling of the specific heat for the 3DIS is very unusual, since all the other critical exponents of the Ising model such as γ and ν decrease uniformly to their mean field values with the increment of dimension from 2 to 4. In 2D it is rigorously proven from the famous solution of Onsager that the scaling behavior of the specific heat is proportional to $\ln t$ ($t \equiv |\beta_c - \beta|/\beta_c$) whereas in 4D, there are several arguments based on the renormalization group equation that the leading order of it is proportional to $(\ln t)^{1/3}$ [5]. Therefore, the the natural estimate of α for the 3DIS is such that the value of α is zero with a certain power of the $\ln t$ between 1/3 and 1. In this dissertation, we will show that indeed this point of view is consistent with the analysis of HTE , of FSS and of the data obtained in the symmetric phase of the 3DIS.

For the HTE analysis of specific heat for the 3DIS, the ratio method assuming no nonanalytic confluent correction will be used. Usually this correction does not make significant difference in the estimate of the critical exponents of the 3DIS(less than 3%). Using Darboux's theorem[7] it was shown that if a function $f(v)$ behaves like

$$f(v) \sim A\left(1 - \frac{v}{v_c}\right)^{-\alpha} + B \tag{5.153}$$

as $v \to v_c$, then in the absence of the competing singularities, one can write

$$f(v) = \sum_{n=0}^{\infty} a_n v^n, \tag{5.154}$$

where the coefficients $\{a_n\}$ satisfy the relation

$$r_n \equiv a_n/a_{n-1} = \frac{1}{v_c}\{1 + \frac{\alpha - 1}{n} + \frac{C}{n^2} + O\left(\frac{1}{n^3}\right)\}. \tag{5.155}$$

Using eq.(5.155) and the data given in the paper of Sykes *et al* [66], $r_n(n = 9, \ldots 14)$ were calculated and the value of v_c , α and the constant C can be immediately estimated as .1024, .2623 and −.7838 respectively using the least square fit. These results are significantly different from those estimated using other methods (here it is between .1 and .125) and from the original estimate by Sykes

et al (α =1/8) obtained by fixing the v_c and C as .10174 and zero respectively. To see how well this ratio method works for other quantitites would be interesting. From the HTE of χ on the FCC lattice[69], the same method with the same range of coefficients(from 9 through 14) was applied to get v_c = .10173 and $\gamma = 1.246$. This result can be compared with the result of McKenzie (v_c =.10173(1) and γ=1.246(5)) who used the Neville table estimates and the result of Guttman[70] (v_c =.10172 γ=1.2427(17)) who used the differential approximants and *included* the non analytic confluent term in his analysis.

Assuming the logarithmic scaling behavior

$$f(v) \sim |\ln[k\left(1-\frac{v}{v_c}\right)]|^{\alpha'}, \tag{5.156}$$

another ratio method based on Tauberian theorem for the estimates of expansion coefficients can be used. The Tauberian theorem[7] can be directly applied to the first derivative of $f(v)$ with respect to v as,

$$f'(v) \sim \left(1-\frac{v}{v_c}\right)^{-1} |\ln[k\left(1-\frac{v}{v_c}\right)]|^{\alpha'-1}. \tag{5.157}$$

As a result of this theorem the expansion coefficient $\{b_n\}$ of $f'(v)$ can be estimated as

$$b_n \sim \frac{Const}{{v_c}^n}\{|\ln\frac{v_c}{n+1}|^{\alpha'-1} + (\alpha'-1)\ln\left(k|\ln\frac{v_c}{n+1}|^{\alpha'-2}\right)\}. \tag{5.158}$$

We define yet another ratio r_n^b as the ratio of b_n and b_{n-1}, then again v_c , α' and k can be easily estimated to be .10163, .81 and 144 respectively from the given $\{b_n\}$. r_8^b through r_{13}^b were used as the input of the modified least square fit. If the series we used is believed to be long enough to give rise to the correct results, from the above result it is evident that logarithmic behavior is much more consistent than that of power scaling. Else, if the series is too short to get a correct result, then it can be said that the power scaling behavior of the 3D specific heat is not supported by the current HTE. To our best knowledge there is no longer series, therefore, it is not possible to clarify this point. Regarding the 3D FSS, we reexamined the data of Barber*et al* [54]. Their FSS data was obtained for β.22165, and we included the

data only with $L \geq 26$ in the analysis. Assuming the power scaling of the specific heat

$$C_V = AL^{\frac{\alpha}{\nu}} + B, \tag{5.159}$$

the value of $\frac{\alpha}{\nu}$ is estimated to be .149 (the original estimate by the authors is .175), meaning that the corresponding value of α is less than .10 with all the currently accepted values of ν. Moreover, it can be easily shown that the data fit a logarithmic function also with almost the same goodness-of-fit(the values of χ^2 are 1.44 and 1.45 respectively). So it seems that the result of FSS study does not really support the power scaling behavior of the specific heat in 3D.

Finally, Monte Carlo simulations have been conducted in the symmetric phase of the 3DIS. We used the single cluster type algorithm originated by U.Wolff [14], and periodic boundary conditions were assumed. First of all, the finite size dependence of magnetic susceptibility (χ), lattice correlation length (ξ) and specific heat (C_v) was investigated at a certain value of β=.210, and the data shows that all these quantities reach the thermodynamic limit already at $L/\xi \simeq 6$. For a given value of β, the averages were taken over six or seven different bins, and typically a bin consists of four or five clusters and one measurement was done per 10 through 20 updating clusters depending on β. As a result, for ξ the statistical error is less than 1% and for the specific heat the statistical error is at most 2%(See Tab(5.14)). We tried to fit the specific heat data to

$$C_v = A(\beta_c - \beta)^{\alpha} + B \tag{5.160}$$

while fixing the β_c value between .2216 and .2217 (β_c is believed to be between .22165 and .22166 by many authors[68]). The result is surprising since the data does not fit, meaning that the fit becomes better and better (the value of χ^2 become smaller and smaller) as the constant B decreases endlessly and at the same time α goes to zero. This is also true with any combination of five different data points from our seven data points. One might try to fit the data with the inclusion of a non analytic confluent term. But as stated before this term does not change the

values of critical exponents by more than 3 % so that it would not effect our final arguments. However these data fit with a logarithmic function

$$C_v = A\{\ln B(\beta_c \ - \beta)\}^{\alpha'} \tag{5.161}$$

with $A \simeq .124$, $B \simeq 34$, $\alpha' \simeq .76$ while fixing $\beta_c \ = .221657$, or $A \simeq .126$, $B \simeq 35$, $\alpha' \simeq .75$ with fixing $\beta_c \ = .221652$. The value of χ^2 is about 6.

Now we discuss an important inequality

$$\alpha \ \geq 2 - D\nu \tag{5.162}$$

which is proven rigorously by Sokal[71]. This inequality shows that for the logarithmic scaling to be correct, the value of ν should be at least 2/3 which is larger than any estimates based on HTE. However, as stated before á priori it is impossible to know whether the series is long enough to yield an accurate result. Here we are talking about a small error typically less than 3%. Therefore, it is not clear whether the existence of the additive confluent term is a *true* one or whether it is present simply to compensate the shortness of the series to yield a consistent estimate of the critical exponents with the hyperscaling. To increase the length of HTE is a very difficult task, therefore, to double the current HTE is almost out of the question. However, Monte Carlo simulations in the symmetric phase of the 3DIS seem to make it possible to produce accurate enough data to clarify this problem.

Table 5.14: 3D Ising data in the symmetric phase. All the values are thermodynamic.

β	L	χ	ξ	C_v
.217	34	130.59(.48)	5.602(.026)	.1979(.0020)
.218	40	176.41(.42)	6.562(.033)	.2155(.0032)
.219	49	263.56(1.37)	8.111(.068)	.2408(.0011)
.220	66	473.12(1.63)	10.939(.046)	.2798(.0019)
.2203	75	607.33(1.13)	12.422(.053)	.2941(.0021)

Table 5.15: Finite size effect study at β =.210.

L	χ	ξ	C_v
12	40.07(.20)	3.024(.010)	.1499(.0005)
15	41.27(.12)	3.064(.010)	.1384(.0008)
18	41.84(.08)	3.085(.007)	.1338(.0008)
21	41.91(.13)	3.093(.012)	.1333(.0011)

Table 5.16: The result of fitting. Here χ^2_χ and χ^2_ξ represent the value of χ^2 for the χ fitting and ξ fitting respectively

β	χ^2_χ	γ	χ^2_ξ	ν
.221645	8.59	1.238	2.44	.639
.221650	6.62	1.242	2.12	.641
.221655	5.12	1.245	1.85	.642
.221660	4.09	1.248	1.59	.644
.221665	3.51	1.252	1.39	.646
.221670	3.36	1.255	1.21	.647
.221675	3.63	1.258	1.06	.649
.221680	4.32	1.262	.948	.650
.221685	5.39	1.265	.862	.652
.221690	6.84	1.268	.805	.654
.221695	8.67	1.271	.776	.655
.221700	-	-	.775	.657
.221705	-	-	.801	.659
.221710	-	-	.852	.660

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