AN ANALOGUE STATISTICAL MECHANICAL APPROACH IN QUANTUM FIELD THEORY

by

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To my parents

"Woran arbeiten Sie?" wurde Herr K. gefragt. Herr K. antwortete: "Ich habe viel Mühe, ich bereite meinen nächsten Irrtum vor."

Bertolt Brecht

ABSTRACT

Scalar and gauge Quantum Field Theories are investigated in the framework of lattice regularisation. Their equivalence to Statistical Mechanical systems allows the implementation of well known Solid State techniques for their study.

In Part A of this thesis, we study the lattice regularised scale covariant $\lambda\phi^4$ scalar field theory. It had been sugested that scale covariant $\lambda\phi^4$, as opposed to canonical $\lambda\phi^4$, may be non-trivial in four dimensions. In order to resolve this question, at least numerically, we investigate the behaviour of the renormalised coupling. With the aid of high temperature series and Pade approximants, we measure the critical index of the renormalised coupling and locate a region of the real parameter space for which its value suggests non-triviality. We then use Monte Carlo simulations to determine the theory's phase diagram. We find that, in the region of the real parameter space where the theory is potentially non-trivial, the transition is first order. The region for which the phase transition is second order, and so the theory possesses a continuum limit is characterised by values of the critical exponent

which imply its triviality . A confluent singularity analysis results in increased numerical accuracy but does not alter the conclusions. We also find that the theory is not incompatible with the notion of universality, although our results are not accurate enough to be conclusive.

Part B is shorter and deals with gauge theories on the lattice. In particular, SU(2) gauge theory is used for a comparative study of the behaviour of Monte Carlo simulations with and without gauge fixing. The axial and the random tree gauge are used. In both cases, and contrary to naive expectations, it turns out that it is advantageous to use Monte Carlo simulations without gauge fixing, because once the gauge is fixed: (a) the system takes longer to thermalise to equilibrium and (b) the error analysis is marginally worse.

PREFACE

The work described in this thesis was carried out in the Theoretical Physics Group of Imperial College, London, between October 1982 and June 1985. Except where otherwise stated, the material is original and has not been submitted before for a degree of this or any other university. The work of Part A of this thesis was carried out under the supervision of Dr. R.J. Rivers. The material of Chapter III, in particular, is the fruit of a collaboration with Dr. N.D. Gent. The work of Part B was supervised by Dr. I.G. Halliday.

I am extremely grateful to my supervisor Dr. R.J.Rivers for suggesting the problems to me, for his help in many (not exclusively academic) matters, for his constant supervision throughout this work and for his friendship. I am also most grateful to Dr. I.G. Halliday for suggesting and supervising the work related to gauge theories as well as helping me in all aspects of this thesis related to the Monte Carlo method.

I would also like to aknowledge the benefit from useful discussions I had with Profs. G. Parisi, J.R. Klauder and B. Lautrup, Drs. N.D. Gent, G.S. Joyce, I.A. Fox, M.R. Lewis and P. Orland and Messrs. R. Brak, M.J. Lavelle and J. Bakas.

Last but not least, I wish to thank Prof. T.W.B. Kibble for encouraging me in many ways to overcome certain difficulties during the early stages of my moving into Physics.

PROLEGOMENA

Lattice spin systems are familiar to most physicists because they model solids which are studied in the laboratory. More recently, such systems have aquired a great importance in a branch of physics which is related to more abstract questions, that of Quantum Field Theory. In particular, space-time lattices are used as a technical device to define cutoff field theories. Eventually, the goal is to define cutoff theories so that field theories defined in real continuum Minkowski space-time can be understood. The lattice is then a mere intermediate regulator used to analyse a difficult non-linear system - a field theory. Thus, once a lattice field theory has been formulated, the original field theory problem becomes one of Statistical Mechanics. This thesis involves a study of certain aspects of the connection of Quantum Field Theories to Statistical Physics. In particular, we observe how the similarity of certain generalised statistical systems to field theory models allows the implementation of well understood solid state techniques in the realm of non-perturbative field theories.

More specifically, the thesis consists of two unequal parts. Part A involves a study of a modified

version of scalar field theories, namely scale covariant $\lambda\phi^4$. This modification was first proposed by Klauder about ten years ago. Essentially it involves a change of measure in the path integral formulation of the theory; whereas conventionally the measure is translationally invariant, Klauder's alternative measure is scale covariant. The motivation and the anticipated consequences of such a change are discussed in Chapter I. It was hoped that this model would give rise to non-trivial $\lambda\phi^4$ theories in d=4 dimensions.

The lattice version of the problem turns out to be a continuous spin Ising model. This enables us to probe the field theoretic behaviour of the system by examining the critical behaviour of the Ising model. It turns out that we are justified in assuming that the renormalised coupling constant of the model has a critical behaviour which is characterised by a critical exponent κ. The sign of κ determines whether the theory's coupling constant approaches a non zero value, vanishes, or diverges near the theory's continuum limit. Thus the sign of κ is a criterion of triviality. This point, together with an exposition of early attempts to investigate the theory, are discussed in Chapter II.

Well understood Solid State techniques such as high temperature series and Pade approximants can be used to obtain values for the critical indices. In this way, it is possible to define regions in the theory's real parameter space for which scale covariant $\lambda\phi^4$ may be a

non trivial-theory. Exploring such a possibility is the first aim of this thesis and is the content of Chapter III.

Such an analysis and the validity of its results, however, presupposes the occurence of a second order phase transition over the whole parameter space. In order to investigate whether this is true, the phase diagram of the theory must be obtained with the use of Monte Carlo simulations. If it turns out that what was an apparent region of non-triviality in the high temperature analysis, lies within a first order phase transition (and thus does not correspond to a continuum field theory) scale covariant $\lambda\phi^4$ will be a trivial theory. Otherwise, non-triviality may arise. This is the second question that this thesis investigates. Chapter IV deals with it.

Also, a more refined study of the theory's subdominant critical behaviour is essential in order to investigate the effect of confluent singularities on the values of the dominant critical exponents. These refinements are neccessary not only for reinforcement of the conclusions on triviality, but also in order to explore whether the theory falls into the same universality class as the values of its real parameters vary. The confluent singularity analysis is the third objective of this thesis. It is carried out in Chapter V.

Part B of the thesis involves another aspect of the

relationship of Quantum Field Theory to Statistical Mechanics; namely that of lattice gauge theories and non-equilibrium statistical behaviour. In particular, gauge fixing in Monte Carlo simulations is expected to alter both the statistical and non-equilibrium properties of the system. A comparative Monte Carlo study of pure SU(2) gauge theory, with and without gauge fixing, is performed in order to see whether gauge fixing is advantageous in aspects of: (a) speed of thermalisation and (b) correlations between measurements which are related to the quality of the statistics. Chapter VI settles such questions. A possible phenomenological explanation for the thermalisation properties is being sought. It is based on the study of the non-equilibrium properties of Monte Carlo simulations in the framework of Stochastic Quantisation.

CONTENTS

PART A

INTRODUCTION

1. Generalities on scalar field theories.

Scalar $\lambda\phi^4_d$ theory (i.e. a field theory with one scalar field ϕ in d spacetime dimensions which has a quartic interaction) has been under intensive study recently. Its study is of interest because according to conventional practice, it has always been regarded as the standard prototype model field theory which shares many extremely essential characteristics with other more physical field theories while remaining considerably simpler than the physical theories. Thus, when considered as a prototype model field theory, $\lambda\phi^4$ serves as testing ground for more physical theories. It is in the framework of $\lambda\phi^4_d$ that our strengths in solving field theories are realised. Similarly, it is in the study of $\lambda\phi^4_d$ that our weakness of a deeper (usually non perturbative) understanding of such theories becomes strikingly apparent.

Moreover, $\lambda\phi^4$ plays an essential part in the spontaneous symmetry breaking mechanism which generates the mass of the gauge particles predicted by unified theories. In particular, the inclusion in the electroweak model's action of a massive scalar particle

with a quartic $\lambda\phi^4$ interaction is essential for the prediction of the correct $W^{\pm}$ and Z masses. Thus, a thorough understanding of a quartic interaction has paramount importance. It is now speculated that there is a radical difference in the properties of a quartic self interaction, depending on whether it is considered on its own or as a sector of a more general unifying theory [1,2]. According to the spirit of this thesis, $\lambda\phi^4$ theories are studied on their own, as a model which, however simple, demonstrates painfully our present lack of profound understanding of field theories. In order to surpass the difficulties, we will attempt to utilise fully its similarity to certain spin systems, the behaviour of which is better understood and for the study of which a rich variety of techniques are already developed.

At present, the problems related to a coherent understanding of $\lambda\phi^4_d$ are numerous. Perturbatively, it is a solvable theory which is superrenormalisable for d=2 and 3, renormalisable in d=4 and nonrenormalisable in $d > 5$ [3]. However, the standard lattice regularisation yields the theory trivial in $d>5$ [4,5,6] , non-trivial in d=2 and 3 [4,5,7,8] and 'almost certainly' trivial in d=4 [6]. This view is supported both by numerical evidence (such as straightforward Monte Carlo computations [9,10,11] and Monte Carlo Renormalisation Group analyses [12,13]) and by series extrapolation techniques based on

high temperature [14,15] and strong coupling expansions (see [16] and references therein). However, this view has been challenged recently from different viewpoints. Non triviality in d=4 arises by using both rigorous [17] and variational [18] techniques which enforce a negative bare coupling constant or, more recently, by an unconventional lattice regularisation and the introduction of 'phantom fields' [19].

However, these last two approaches were not the only ones to render the theory non-trivial in d=4. A more radical approach was based on the idea that the pathologies of $\lambda\phi^4$ might arise at a very early stage, namely from the conventional (canonical or path integral) quantisation of field theories. The situation could be remedied by adopting an alternative quantisation scheme which is known as Scale Covariant Quantisation. The resulting scale covariant theories are considerably different from the canonical ones and can be thought of as their generalisation. It may be noted at this early stage that earlier work on scale covariant field theories was also pointing in the non-triviality direction. Clearly, such a controversial situation cries out for a careful analysis and a thorough testing of the validity of any underlying assumptions on which the final results depend. Since scale covariance is a fundamentally different approach to canonical quantum field theories, we will devote the first chapter to its motivation.

CHAPTER I

INTRODUCING SCALE COVARIANCE

1. Generalities on scale covarince

Scale covariant field theories have been proposed by Klauder [10] as a formal quantisation scheme (alternative to conventional field theories) which has two ambitions: (a) give a physical interpretation to theories which perturbatively are non-superrenormalisable and (b) cure certain field theories from their triviality. Given the problematic condition of the present day status of field theories as presented in the introduction, one is clearly tempted to consider alternative quantisation schemes that might not have these problems.

Motivating Scale Covariance field theories can be tedious. The scheme does not arise naturally. The main ideas can be more clearly presented through examples of both quantum mechanical and field theoretic models. This is in accordance with the the spirit of the whole history of its development: Scale Covariance has arisen as an alternative scenario to canonical quantisation based on plausibility arguments rather than rigourous results. What follows is a description of the most important steps of the whole motivation ; no proofs will be given.

2. Discontinuous perturbations in Quantum Mechanics

The first crucial observation in what might be wrong in conventional approaches is the discovery of a class of quantum mechanical models which do not satisfy the most fundamental assumption of perturbation theory which states that if a Hamiltonian H can be decomposed into a free part H_o and an interaction λV like :

$$H = H_o + \lambda V \tag{1.1}$$

then as $\lambda \to 0^+$, $H \to H_o$. The eigenfunctions and eigenvalues of H pass continuously to those of H_o in the same limit. This is the conventional picture and we shall refer to it as continuous perturbation.

Although such continuity seems obvious enough, counterexamples exist for certain impenetrable interactions V. In such cases, as $\lambda \to 0^+$,

$$H \to H_o' \neq H_o \tag{1.2}$$

If this is the case, then the eigenfunctions and eigenvalues of H pass continuously to those of H_o' but not to those of H_o ; they remain disconnected from the solutions of the free theory. We shall call H_o' the

pseudofree Hamiltonian. H is continously connected to H_o' but not to H_o. Thus, standard perturbations are expected to fail, because they attempt to solve the problem by developing their solutions around H_o, which is disconnected from the fully interacting Hamiltonian H. This situation has been termed discontinuous perturbation by Klauder [20] who proposed it as a conceivable parallel to nonrenormalisability. On the contrary, continuous perturbations around the pseudofree theory ought to produce meaningful calculations.

Klauder [21] has demonstrated his point by considering the following specific Hamiltonian in one dimension (d=1) :

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{\lambda}{|x|^\alpha} \qquad (1.3.a)$$

This model can be tackled directly [21,22]. It turns out that for any $\alpha < 1$, $H \to H_o'$ as $\lambda \to 0^+$ and the potential is a continuous perturbation of H_o. For $1 \leq \alpha < 2$, one must first regularise V and then remove the regularisation with the use of counterterms [23] before arriving to the same conclusion. When $\alpha > 2$ however, and when the potential becomes impenetrable, such a regularisation does not exist. The limit $\lambda \to 0^+$, enforces H to a pseudofree Hamiltonian

$$H_o' = -\frac{1}{2}\frac{d^2}{dx^2}\Big|_{DBC} + \frac{1}{2}x^2 \qquad (1.3.b)$$

where DBC stands for Dirichlet boundary conditions. This means that $\psi(0) = 0$; i.e. the impenetrability of V at x=0 enforces the Hamiltonian and its solutions ψ to "remember" the interaction even after its presence has been removed. The first four eigenfunctions and eigenvalues of both H_o and H_o' are shown in Figure (1.1). Upon reintroduction of the perturbation we find that the energy levels of H depart continuously from those of H_o'. More specifically, if E_n' are the energy levels of the pseudofree Hamiltonian, the energy levels of H are (for small λ)

$$E_n' + O(\lambda) \quad \text{for } 2 < \alpha < 3 \qquad (1.4.a)$$

$$E_n' + O(-\lambda \ln\lambda) \quad \text{for } \alpha = 3 \qquad (1.4.b)$$

$$E_n' + O(\lambda^{1/(\alpha-2)}) \quad \text{for } \alpha > 3 \qquad (1.4.c)$$

3. Discontinuous perturbations and path integrals

The previous picture has a corresponding description in the path integral formalism. As is well known, the transition amplitudes of any theory defined by its action

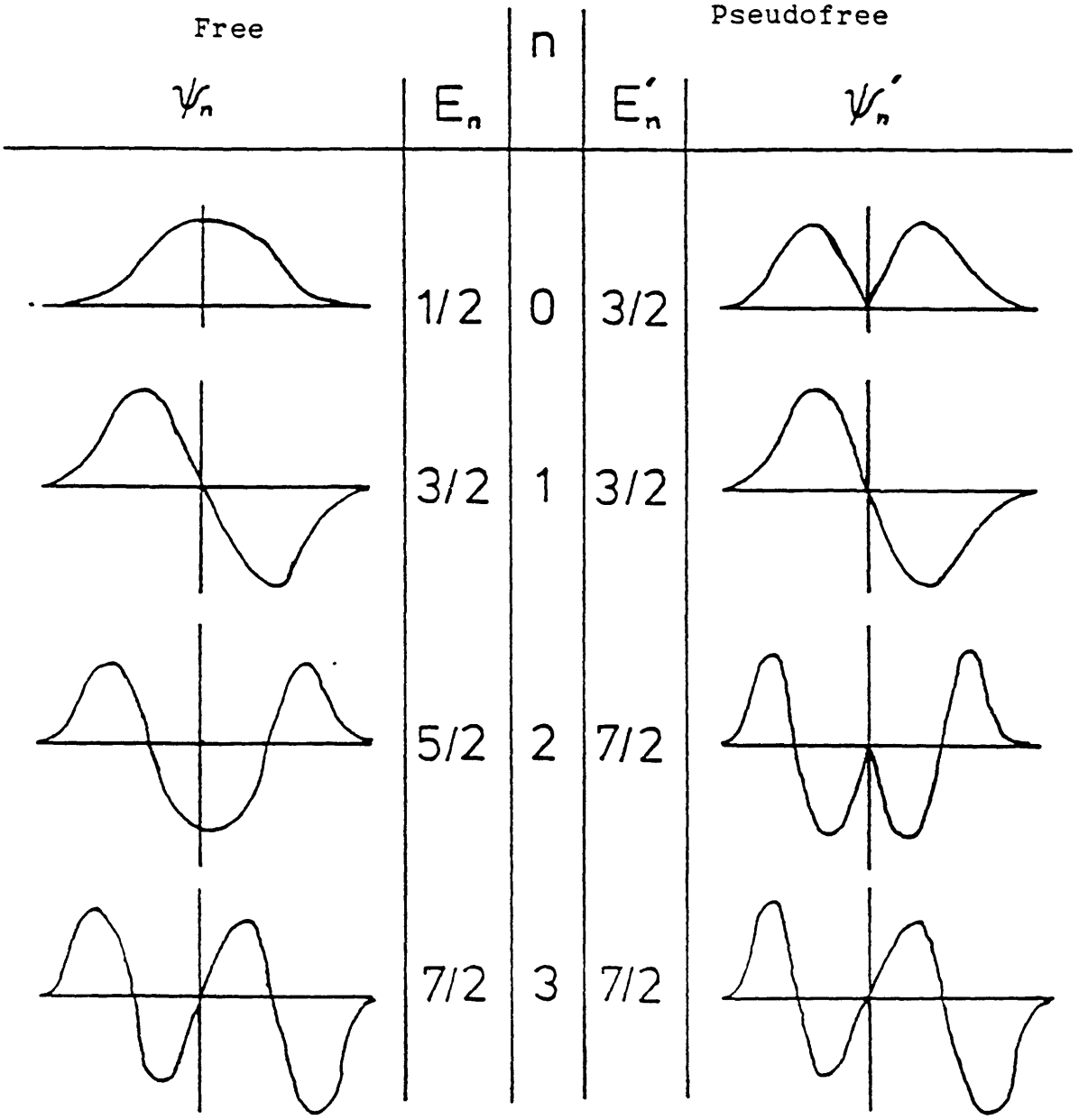


FIG. 1.1 : First four wavefunctions and energy levels for the harmonic oscillator and the pseudofree oscillator H_o'

S can be obtained from a path integral which can be formally written as.

$$Z = \sum_{\text{paths}} \exp(-iS) \tag{1.5}$$

where the summation is over all paths between the initial and final points in phase space. Now the action splits up into two parts analogous to those of eq. (1.1)

$$S = S_o + S_I \tag{1.6}$$

The free theory is then described by

$$Z_o = \sum_{\text{paths}} \exp(-iS_o) \tag{1.7}$$

However, Klauder has pointed out that the paths involved in the summation of (1.5) may be different to those of (1.7) [20]. The presence of a singular interaction S_I in (1.5) may act as a partial hard core, projecting out from the summation those paths that are suppressed by it. For example, for the model defined by (1.1), equation (1.5) becomes the standard Feynman path integral

$$Z = N \int Dx(t) \exp\{-i \int dt \left[\frac{1}{2}\dot{x}^2 + \frac{1}{2}x^2 + \frac{\lambda}{|x|^\alpha}\right]\} \tag{1.8}$$

and the presence of the interaction suppresses all paths which for any time t can be x(t)=0. If now $\lambda \to 0^+$ these

paths remain projected out and the resulting Z_o' is different from that of the free theory's, Z_o, which includes contributions from the suppressed paths. It may be noted that the above is only a plausibility argument. In Section 4 of this chapter, a slightly more accurate analogue will be exposed in terms of a field theory. The message however, is already quite clear : Once an impenetrable interaction is switched on, it cannot be turned off by diminishing its coupling strength.

Before proceeding from Quantum Mechanics to Field Theory, we believe that a crucial observation is in place. We see that eqn. (1.8) gives for the dimension of λ

$$\text{dim } \lambda = \text{dim (length)}^{\alpha-2} \qquad (1.9)$$

Thus, for dim λ = dim(length)$^{-ve}$ ($\alpha < 2$) the free theory is connected to H, whereas for dim λ = dim(length)$^{+ve}$ ($\alpha > 2$), H is disconnected from H_o. The coupling λ is dimensionless for the critical case $\alpha = 2$. It may be noted that the dimensionality of the coupling constant serves as a criterion for the renormalisability of field theories, since for, say, scalar $\lambda\phi^p$ we have

$$\text{dim } \lambda = \text{dim(length)}^{p-4} \qquad (1.10)$$

Although coupling constant dimensionality is not

invariably a correct guide to such behaviour, the connection is of obvious interest.

4. The Independent Value Model (IVM)

So far the discussion was limited to Quantum Mechanics. We will now expose the same ideas for field theories. The style of presentation will not be altered: The main ideas will be exposed through a specific example and the results will be stated without proof. The example in question is a toy model developed by Klauder [24] called the Independent Value Model (IVM). In Euclidean space it is formally defined by the path integral

$$Z(h) = N \int d\phi \exp \{ \int dx \, (ih\phi - \frac{1}{2} m^2 \phi^2 - \lambda \phi^p) \} \quad (1.11)$$

Two basic characteristics of the model can be readily read off from (1.11) : (a) The lack of gradients of the field implies no propagation ; thus the IVM is of mathematical rather than of physical interest. (b) The IVM is severely nonrenormalisable, as can be seen by naive power counting (we shall examine here the p=4 case).

The independent behaviour of each space-time point enabled Klauder [21] to show that (1.11) can be written in the canonical form (for p=4)

$$Z(h) = \exp\left\{-b \int dx \int \frac{du}{|u|} [1-\cos(hu)]\, e^{-1/2\ bm^2 u^2 - \lambda b u^3 u^4}\right\} \tag{1.12}$$

with b an arbitrary positive constant. The limit $\lambda \to 0^+$ gives rise to the solution

$$Z_o'(h) = \exp\left\{-b \int dx \int [1-\cos(hu)]\, e^{-1/2\ bm^2 u^2} \frac{du}{|u|}\right\} \tag{1.13}$$

which is a pseudofree theory, since it is distinct from the free theory. The free theory can be obtained from equation (1.11) by putting $\lambda \equiv 0$ and has the form

$$Z_o(h) = \exp\left\{-B \int dx\ h(x)^2\right\} \tag{1.14}$$

($B \geq 0$ an arbitrary constant). The zeroth order term in a perturbative expansion of (1.12) is (1.13) and not (1.14).

Moreover, Klauder has shown that from (1.12), it can be derived that the connected part of all even order correlation functions are non-negative

$$\langle \phi(x_1)\ \phi(x_2)\ \phi(x_3)\ \phi(x_4) \rangle_c \geq 0 \tag{1.15}$$

This is a very important result, as we shall see in the following section.

5. The IVM on the lattie

An interesting situation arises if we regularise the IVM by defining it on a lattice. Given any continuum field theory, we can assume it has an equivalent Euclidean lattice space form. The conventional way of approximating the continuum with a d-dimensional, hypercubic, isotropic lattice with lattice spacing a, is to introduce the following changes :

$$x \to ak \quad (k \text{ integer}) \tag{1.16.a}$$

$$\int dx \to \sum_{d} a^{d} \tag{1.16.b}$$

$$\phi(x) \to \phi_{k} \tag{1.16.c}$$

in terms of which , the lattice regularised IVM becomes:

$$Z(h_{s}) = N \int \prod_{s} d\phi_{s} \exp\{-S[\phi,h]\} \tag{1.17.a}$$

where S is the lattice action

$$S[\phi,h] = \sum_{s} \left(\sum_{d} 1/2\ m_{o}^{2} a^{d} \phi_{s}^{2} + \lambda_{o} a^{d} \phi_{s}^{4} - i h_{s} \phi_{s} \right) \tag{1.17.b}$$

This formulation, however, has the disadvantage that it

belongs to a class of models which satisfy the Lebowitz inequality [25]

$$\langle \phi_s \phi_k \phi_l \phi_t \rangle_c \leq 0 \qquad (1.18)$$

This is true even in the limit $a^d \to 0$,so the only way it will not contradict (1.15) is for the four point function to vanish. Thus, the continuum renormalised theory which can be recovered from the lattice IVM of (1.17) is the free theory Z_o of (1.14).

The pseudofree theory can only be recovered if we define the following lattice version for the IVM :

$$Z(h) = N \int \prod_s \frac{d\phi_s}{|\phi_s|^{1-2ba^d}} \exp\{-S[\phi,h]\} \qquad (1.19)$$

with the action as in (1.17.b). As has been shown by Klauder [20], when $a^d \to 0$, the interacting continuum theory (1.12) is obtained.

The important observation from such manipulations is the fact that in order to recover the exact solutions of the IVM, we were forced to introduce a new measure

$$D_B \phi_t \equiv \prod_t \frac{d\phi_t}{|\phi_t|^B} \qquad (1.20.a)$$

($B \equiv 1-2ba^d$) which is radically different from the

conventional measure

$$D\phi_t \equiv \prod_t \phi_t \qquad (1.20.b)$$

The new measure is scale covariant, i.e. under a field scaling

$$\phi_t \to \Lambda_t \, \phi_t \qquad (1.21.a)$$

with

$$\Lambda_t > 0 \qquad (1.21.b)$$

it transforms covariantly

$$D_B\phi \to F(\Lambda) \, D_B\phi \qquad (1.22)$$

($F(\Lambda) = \prod_t |\phi_t|^{-B}$ is a scaling factor) as opposed to the conventional measure which under field translations

$$\phi_t \to \phi_t + \Lambda_t \qquad (1.23.a)$$

remains invariant :

$$D \, \phi_t \to D \, \phi_t \qquad (1.23.b)$$

In the continuum limit, $B \to 1$ and the measure $D_1\phi$ becomes

scale invariant, i.e. it remains invariant under scaling of the form (1.21.a)

$$D_1\phi \to D_1\phi \tag{1.24}$$

In conclusion, we argue that a common characteristic which is shared by the IVM and the previously examined quantum mechanical example is not only a pseudofree theory which is disconnected from the free one, but also, to a certain extent, the scale covariance property. In the following section, we shall examine how it is possible for such considerations to affect properly propagating scalar field theories.

6. Discontinuous perturbations and scalar $\lambda\phi^p$ field theories

Having examined two simple models for which the main ideas work out exactly, we shall speculate on how the same principles can be applied to the more interesting $\lambda\phi^p$ field theory (with special attention to the p=4 case). The action of the theory in Euclidean space-time is (in d dimensions)

$$S(\phi,h) = \int d^dx \{1/2 (\partial_\mu\phi)^2 + 1/2\, m_o^2\phi^2 + \lambda_o\phi^p - ih\} \tag{1.25}$$

and its canonical path integral quantisation is provided

by the generating functional

$$Z(h) = N \int D\phi \exp(-S) \qquad (1.26)$$

where the functional measure is conventionally thought to be

$$D\phi = \prod_x d\phi(x) \qquad (1.27)$$

The action has a free part

$$S_o(\phi,h) = \int d^dx \{1/2 (\partial_\mu \phi)^2 + 1/2 m_o^2 \phi^2 + - ih\phi\} \qquad (1.28.a)$$

and an interacting part

$$S_I(\phi) = \int d^dx \lambda\phi^p \qquad (1.28.b)$$

Thus, the generating functional can be written as

$$Z(h) = N \int D\phi \exp(-S_o - \lambda_o S_I) \qquad (1.29)$$

and the free generating functional as

$$Z_o(h) = N \int D\phi \exp(-S_o) \qquad (1.30)$$

The requirement of perturbative analyses is that λS_I is controllably small for small λ ; i.e. when $\lambda \to 0^+$, S

reduces to S_o. For this to be true we must ensure that $|S_I|$ is bounded when S_o is bounded so that the path integral (1.29) can be regarded as a summation over all paths for which S_o (and S) are finite. This being true, Z can be solved as a perturbation of Z_o. If, however, there are paths for which $|S_I|$ is unbounded while S_o is not, canonical perturbation series are expected to fail. In order to get sensible perturbation series for an S_I which can be unbounded, we need to excise those paths for which S_I is uncontrollable and thus impose a path integral summation over this subset of the paths that keep S_o finite, for which S_I also stays finite.

One can formalise this situation by the following argument [26]. The relevant measures of the theory are postulated to be

$$d\mu(\phi) = \exp(-S)\, D\phi\, \chi \qquad (1.31.a)$$

for the interacting, and

$$d\mu_F(\phi) = \exp(-S_o)\, D\phi \qquad (1.31.b)$$

for the free case. We have introduced an indicator function $\chi(\phi)$ such that

$$\chi(\phi) = 1 \text{ when } S_o(\phi) < \infty \text{ and } S_I(\phi) < \infty \qquad (1.32.a)$$

$$\chi(\phi) = 0 \text{ when } S_o(\phi) < \infty \text{ and } S_I(\phi) = \infty \qquad (1.32.b)$$

The generating functional is now defined to be

$$Z(h) = \int d\mu(\phi)\, \exp(i \int h\phi\, d^d x) \qquad (1.33)$$

It is suggestive that, as $\lambda \to 0^+$,

$$d\mu(\phi) \to \chi(\phi)\, d\mu_F(\phi) \equiv d\mu_{PF}(\phi) \qquad (1.34)$$

with $d\mu_{PF}(\phi)$ the measure of the pseudofree theory. According to (1.32), (1.34) means that for certain interactions the relative supports of the free and interacting theory can be dissimilar, so as $\lambda \to 0^+$, the interacting theory passes to a pseudofree one. This discussion demonstrates the necessity for a change of measure that will explicitly generate the above "path suppression" mechanism.

Although the above argument may sound convincing, it has only rudimentary value, since paths for which the action is finite, give zero contribution to the generating functional. Only configurations of infinite action have non-zero measure. Given this, Klauder [21,26] has sressed that the above must be thought of as a kind of "zeroth order" formalism and can only be a good guide to the relative supports of the measures.

The formal change of measure involving the introduction of the indicator function $\chi(\phi)$ is not arbitrary. It must be compatible with some kind of equal time commutation relationships (ETCR), just like the canonical measure is equivalent to the canonical ETCR's. The argument is heuristic and can be described in broad lines as follows: Recall that for the canonical case, postulating the classical equation of motion and tha ETCR's gives rise to the Swinger-Dyson (S-D) equation (for p=4)

$$\{h(x) + (m_0^2-\nabla_x^2) \frac{\delta}{\delta h(x)} - 4\lambda_0 \frac{\delta^3}{\delta h(x)^3} \} Z(h) = 0 \qquad (1.35)$$

This equation can also be obtained as a result of the principle of translational invariance of the theory. If we want both the measure and the action to be invariant under field translations

$$\phi(x) \rightarrow \phi'(x) = \phi(x)+\Lambda(x) \qquad (1.36)$$

then we must ensure that

$$\frac{\delta}{\delta\Lambda(x)} Z(h)_\Lambda \Big|_{\Lambda=0} = 0 \qquad (1.37)$$

where $Z(h)_\Lambda=Z(h)$ is the generating functional expressed in terms of translated fields $\phi'(x)$. Written explicitly,

eqn. (1.37) in no other but eqn. (1.35).

In trying to determine the pseudofree measure of equation (1.34) in a fashion which is consistent with some ETCR's, we have very litle to build upon. In particular, we can only rely on the only tangible results we have concerning the IVM and on the analogies to the previous arguments governing canonical field theories. If, guided by our results for the IVM, we impose covariance under field scaling

$$\phi(x) \rightarrow \phi'(x) = \Lambda(x)\phi(x) \tag{1.38}$$

the scale covariant measure must satisfy

$$D_{SC}\phi'(x) = F(\Lambda)\, D_{SC}\phi(x) \tag{1.39}$$

Since the same must be true of the path integral, the analogous relationship to (1.37) is

$$\frac{\delta}{\delta\Lambda(x)} \; Z_{SC}(h)_{\Lambda} \; \Big|_{\Lambda=1} = 0 \tag{1.40}$$

with $Z_{SC}(h)_{\Lambda}$ the generating functional with scaled fields. This gives rise to the modified S-D equation

$$\{h(x)\frac{\delta}{\delta h(x)} + :\frac{\delta}{\delta h(x)}(m_0^2 + \nabla_x^2)\frac{\delta}{\delta h(x)}: - 4\lambda_0 :\frac{\delta^4}{\delta h(x)^4}:\}Z_{SC} = 0 \tag{1.41}$$

with

$$:\frac{\delta^p}{\delta h^p(x)}: Z_{SC} \equiv \frac{\delta^p}{\delta h^p(x)} Z_{SC} - \frac{\delta^p}{\delta h^p(x)} Z_{SC}\Big|_{h=0} Z_{SC} \quad (1.42)$$

It turns out [29] that the simplest choice of measure that satisfies (1.39) is

$$D_{SC}\phi(x) = \prod_x \frac{d\phi(x)}{|\phi(x)|^B} \quad ; \quad B < 1 \quad (1.43)$$

Having argued that our choice of measure (1.43) gives rise to a modified S-D equation, we must also check that eqn. (1.41) can also be obtained [20] from a modified version of ETCR's. These are the affine commutation relationships. They read

$$[\tfrac{1}{2}\{\pi(x),\phi(x)\} , \phi(y)] = -i \phi(x) \delta(x-y) \quad (1.44)$$

At this point, it is interesting to state briefly that Klauder pointed out the existence of a Sobolev-type inequality [20,21]

$$\frac{|S_I^2|^{\frac{1}{2}}}{|S_o|} < K \quad ; \quad \forall\phi \quad (1.45)$$

for $d<4$ (K is a finite constant). This is obviously

equivalent to saying that $|S_I| < \infty$ when $|S_O| < \infty$. Thus, for $d<4$ there is no motivation for a change of measure from this viewpoint. Thus, we see that superrenormalisability is somehow related to the Sobolev-type topological equivalence of the interacting and free theories. It is in $d>4$ (and $d=4$ as a borderline case) that the motivation for a change of measure may be connected to the problematic state of the renormalisability and triviality of the canonical theories.

Thus, by an amalgam of exact results and analogies to canonical field theories, Klauder has managed to propose an alternative quantisation scheme. It essentially involves the introduction of the scale parameter B in the new measure of the path integral, as defined by equation (1.43). Note that we must ensure that $B < 1$, for the path integral to converge. When $B = 1$, the theory becomes scale invariant. In the $B = 0$ case, the canonical theory is retrieved as a special case of scale covariance, and when $\lambda \to 0^+$ (with $B \neq 0$) a pseudofree theory, distinctly different from the free one is recovered. This modification of the measure gives rise to an alternative quantisation scheme which involves new ETCR's and S-D equations.

Since all these ideas have worked for the IVM, it is worthwile to try them out for more physical theories. It is possible that in asymptotically free

superrenormalisable theories the free and pseudofree solutions coincide and perturbative evaluations around the free solution are in place. However non-asymptotically free,nonrenormalisable and (as a limiting case) renormalisable theories have pseudofree solutions that are disconnected from the free case and perturbative expansions ought to be carried out around the pseudofree solution. These ideas have been successfully applied to the O(N) symmetric $\lambda\phi^4$ model and they appear to work in the large N limit [30,31,32,33,34].

However this is not the end of the story. If non-asymptotically free, non-renormalisable and renormalisable theories are to be rectified by scale covariance, their lattice regularisation should better not render them trivial. That scale covariant theories should have non-trivial solutions is the most important consequence of the previous arguments. This is the most investigated aspect in recent research on scale covariant theories. The rest of Part A of this thesis deals precisely with this problem. Early work in this direction was encouraging. It has been shown that for certain fine 'tunings' of B in the large N limit, the O(N) symmetric $\lambda\phi^4$ theory becomes non trivial [35,36]. Also, a numerical study of the lattice pseudofree theory showed evidence of non triviality [29]. We shall refer to this last work in detail.

Having motivated the concept of scale covariance, we

will now proceed to a detailed discussion of the properties it has once it is expressed in the framework of lattice regularisation.

CHAPTER II

LATTICE FORMULATION OF SCALE COVARIANT FIELD THEORY

1. Definition of the theory on the lattice

In the previous Chapter, we have shown that scale covariance, an alternative quantisation scheme, may rectify certain problems that appear in canonically quantised field theories. The continuum scale covariant version of $\lambda\phi^4$ is defined by the generating functional [29]

$$Z[J] = N \int [D_B\phi] \exp\Big(i\int d^dx \Big\{\frac{1}{2}(\partial_\mu\phi)^2 - \frac{1}{2} m_o \phi^2 - \lambda_o\phi^4 - J\phi\Big\}\Big) \qquad (2.1)$$

with measure

$$D_B\phi \equiv \prod_x \frac{d\phi(x)}{|\phi(x)|^B} \quad ; \quad \forall x \qquad (2.2)$$

In the previous Chapter, the lattice approximation of field theories was introduced as an essential step for a complete understanding of the basic properties of the

IVM. Although the solution of the model could be obtained while remaining in the realm of continuum physics, its aspects related to the triviality question could only be studied through the lattice approach. This is hardly surprising since the triviality aspects for canonical $\lambda\phi^4$ field theory were always apparent in the framework of lattice regularisation. It is therefore natural to consider the lattice formulation of scale covariant $\lambda\phi^4$. As we pointed out in Chapter I, the lattice regularisation may be introduced through the changes expressed in (1.16) together with the introduction of a lattice equivalent for derivatives, namely

$$\partial_\mu \phi(x) \rightarrow \frac{1}{a} (\phi_i - \phi_{i+\underline{\mu}}) \qquad (2.3)$$

where $\underline{\mu}$ is a vector of length a in the μ direction. In terms of (1.16) and (2.3), we may now express the lattice analogue of the model in d Euclidean dimensions. It is generated by

$$Z[J] = N \int [\prod_k \frac{d\phi_\kappa}{|\phi_k|^B}] \exp(- S[\phi] - \Sigma\, a^d J_k \phi_k) \qquad (2.4)$$

with action

$$S[\phi] = \frac{1}{2} \sum_{k} \sum_{\mu=1}^{d} a^{d-2} (\phi_k - \phi_{k+\mu})^2 +$$

$$+ \frac{1}{2} \sum_{k} a^d m_o^2 \phi_k^2 + \sum_{k} a^d \lambda_o \phi_k^4 \qquad (2.5)$$

Note that apart from the new measure, expressions (2.1), (2.4) and (2.5)) are identical to those of canonical $\lambda\phi^4_d$. The effect of the new measure is expressed by the introduction of the scaling parameter B. This increases the real parameter space by an extra dimension. Whereas the canonical theory's real parameter space as defined by the pairs of bare parameter values (m_o, λ_o) is two dimensional, we now have a three dimensional parameter space spanned by (m_o, λ_o, B). Now, standard $\lambda\phi^4_d$ will be recovered as a special case of scale covariance by setting $B \equiv 0$.

We use the standard equivalence of $\lambda\phi^4$ to a spin ferromagnet [18] by reparametrising the model. In particular, we may redefine : (i) a new dimensionless field (which will be shortly shown to be like a continuous classical spin degree of freedom of a statistical mechanical Ising-like spin system) in terms of the old field ϕ and a dimensionless scaling parameter K

$$\sigma_k = \frac{a^{(d-2)/2}}{\sqrt{K}} \phi_k \qquad (2.6.a)$$

(ii) a new "mass" parameter A in terms of the old bare mass m_o and K

$$A = (d + \frac{m_o^2 a^2}{2}) K \qquad (2.6.b)$$

(iii) a new bare coupling constant U_o in terms of the old one λ_o and K

$$U_o = a^{4-d} K^2 \lambda_o \qquad (2.6.c)$$

and (iv) a new external source h in terms of the old one J and K

$$h_k = \sqrt{K}\, a^{(2-d)/2} J_k \qquad (2.6.d)$$

This change of variables maps the three parameters (B, m_o, λ_o) into four (B, A, U_o, K). In order to remove the one extra parameter, we may impose a normalisation condition similar to mass renormalisation [15].

$$\frac{\int \frac{dx}{|x|^B}\, x^2 \exp (- A x^2 - U_o x^4)}{\int \frac{dx}{|x|^B} \exp (- A x^2 - U_o x^4)} = 1 \qquad (2.7)$$

This equation can in principle be solved to give A as a function of B and U_o. In practice this is done numerically ; i.e. given the values of B and U_o, one can solve (2.7) numerically for A, by using existing software library packages for finding zeroes of functions and for numerical integration. Thus, A can be plotted as a function of U_o for different values of B (see Figure (2.1), which is reproduced from Ref. [37]). We have used the NaG 8 Fortran Library for these numerical manipulations.

The partition function is now given by

$$Z[h] = N' \int \prod_k d\mu(\sigma_k) \exp (- S[\sigma]) \qquad (2.8)$$

with action

$$S[\sigma] = - K \sum_k \sum_{\mu=1}^{d} \sigma_k \sigma_{k+\mu} + \sum_k \sigma_k h_k \qquad (2.9)$$

and single site spin distribution

$$d\mu(\sigma_k) \equiv \frac{d\sigma_k}{|\sigma_k|^B} \exp(- A \sigma_k^2 - U_o \sigma_k^4) \qquad (2.10)$$

Note that the integrals of (9) are well defined only for $B < 1$. Obviously, the action is now that of a continuous spin Ising model with inverse temperature K and external

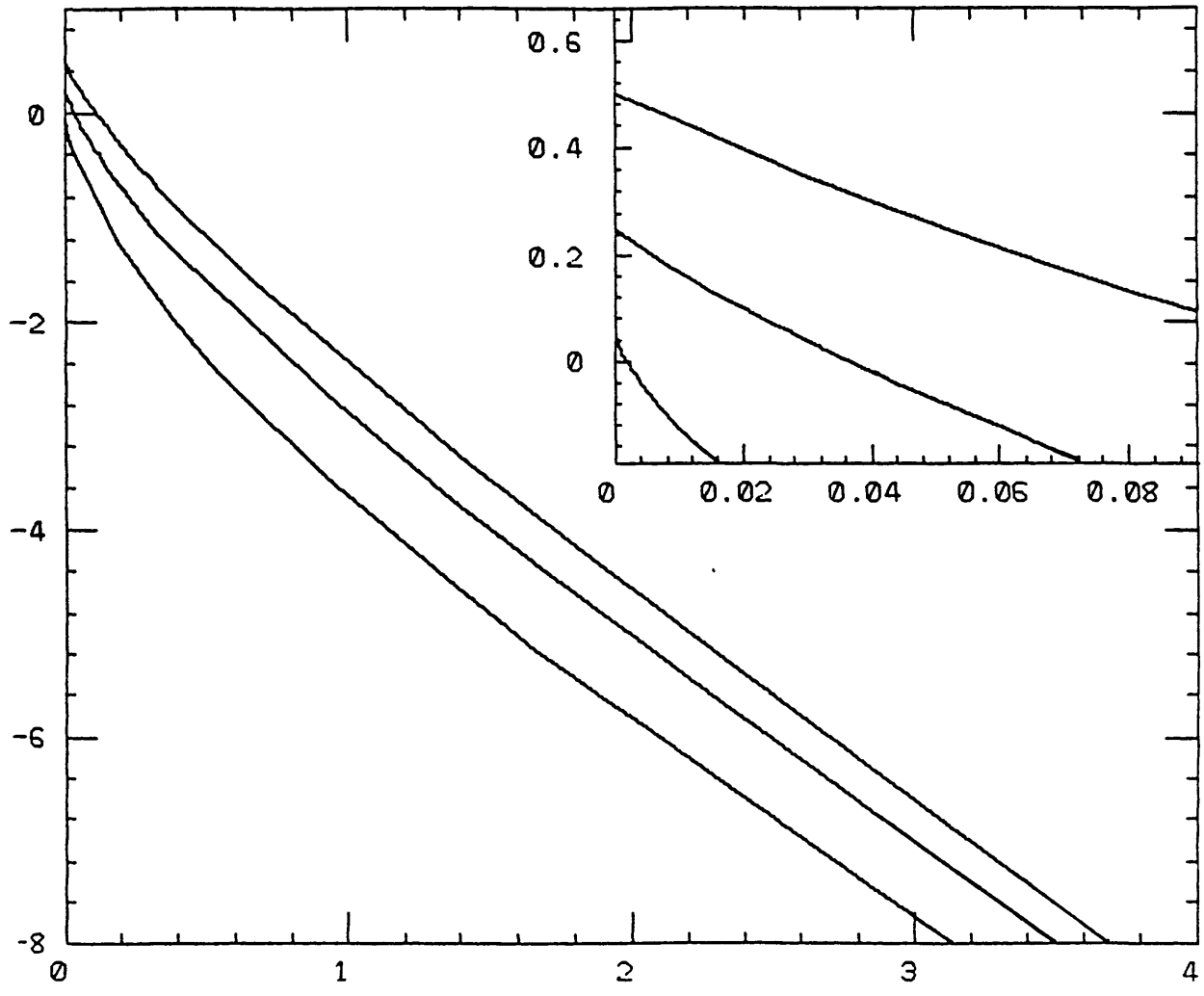


FIG. 2.1 : The normalised mass parameter $A(B,U_o)$ as a function of U_o for B=0 (upper curve) , B=0.5 (middle curve) and B=0.9 (lower curve). Insert : magnified view of the behaviour near $U_o=0$.

magnetic field h. Given this, we will from now on adhere to a statistical mechanics rather than a field theory language and define spin correlations by

$$\langle \prod_k \sigma_k \rangle \equiv Z[h]^{-1} \int [\prod_i d\mu(\sigma_i)] [\prod_k \sigma_k] \exp(- S[\sigma]) \qquad (2.11)$$

Using this definition, we now introduce those correlation functions which we will subsequently use in our study. They are : the susceptibility

$$\chi \equiv \sum_k \langle \sigma_o \sigma_k \rangle_c \qquad (2.12.a)$$

the fourth cumulant

$$\chi_{(2)} \equiv \sum_{klm} \langle \sigma_o \sigma_k \sigma_l \sigma_m \rangle_c \qquad (2.12.b)$$

and the second moment of the spin-spin correlation function

$$\mu_2 \equiv \sum_k \frac{k_\mu k_\mu}{a^2} \langle \sigma_o \sigma_k \rangle_c \qquad (2.12.c)$$

where c denotes the connected part. In terms of these thermo- dynamical quantities we can now define the dimensionless correlation length

$$\xi \equiv \left(\frac{\mu_2}{2d\chi} \right)^{1/2} \qquad (2.13.a)$$

and the dimensionless scale invariant renormalised coupling constant

$$g_R \equiv - \frac{\chi_{(2)}}{\xi^d \chi^2} \qquad (2.13.b)$$

2. Continuum limit and critical behaviour

We have expressed the original lattice regularised field theory as an equivalent continuous spin Ising model. However, since it is the continuum field theory that we are ultimately interested in, the continuum limit of the statistical system must be carefully considered.

Since the model is regularised by a lattice of spacing a, one must take the $a \to 0$ limit in order to arrive to continuum physics. This is a highly non-trivial limit as it must be taken while keeping certain physical quantities fixed. In particular, one must renormalise the bare parameters and thus express the dressed physical parameters as functions of the bare ones. For example, in the canonical theory one must in principle have the dependences [3,38]

$$m_R = m_R(m_o, g_o, a) \qquad (2.14.a)$$

$$g_R = g_R\,(m_o,\ g_o,\ a) \qquad (2.14.b)$$

and whenever the limit $a \to 0$ is taken, m_R must be held fixed to the value of some physical mass. Recall that m_R is given by the exponential behaviour of the two point Green' s function at large physical distances $x = ak$, where k is the distance in lattice units, i.e. [38,39]

$$G(0,x) \sim \exp(-m_R x) = \exp(-m_R ak) \qquad (2.15.a)$$

From the theory of spin systems we know that the spin-spin correlation function for largely separated spins is given by [39]

$$G(0,k) \sim \exp(-k/\xi) \qquad (2.15.b)$$

Thus, we obtain the all important relationship

$$m_R \xi a = 1 \qquad (2.16)$$

where ξ is measured in lattice units a.

Clearly, the only way this relationship can be true in the continuum limit ($a \to 0$) while m_R is kept at a fixed physical value is for the correlation length ξ to diverge. However, $\xi \to \infty$ is the conventional signal for a second order phase transition [40]. Thus, when the statitistical mechanical system displays a second order phase transition, the equivalent lattice field theory

approaches its continuum limit. This is why we are primarily interested in the critical region of the system, characterised by the divergence of ξ. Assuming the existence of a second order phase transition at a critical inverse temperature K_c, the dominant critical behaviour of the quantities of interest is given by :

$$\chi = f_1(K)\ (K_c-K)^{-\gamma} \qquad (2.17.a)$$

$$\chi_{(2)} = f_2(K)\ (K_c-K)^{-\gamma-2\Delta} \qquad (2.17.b)$$

$$\mu_2 = f_3(K)\ (K_c-K)^{-\gamma-2\nu} \qquad (2.17.c)$$

$$\xi = f_4(K)\ (K_c-K)^{-\nu} \qquad (2.17.d)$$

$$g_R = f_5(K)\ (K_c-K)^{\kappa} \qquad (2.17.d)$$

with

$$\kappa \equiv d\nu + \gamma - 2\Delta \qquad (2.18)$$

Here the $f_i(K)$ $(i=1,\ldots,5)$ are assumed to be analytic functions in the region of K_c, neglecting $\ell n(K_c - K)$ terms and confluent power singularities. So, as $K \to K_c^-$, the dominant divergence is that of the critical exponent of the $K_c - K$ term.

For our study, the value of κ is most important. If $\kappa > 0$, $g_R \to 0$ as $K \to K_c^-$ and the theory is trivial. If $\kappa < 0$, g_R diverges at K_c and this is considered a signal for the non existence of a continuum field theory [41]. So for the theory to be non trivial in the continuum limit, g_R must assume a non- zero value, which is only possible if $\kappa = 0$. In order to investigate the problem of triviality, we first need a method of evaluating the quantities of eqns. (2.17) as functions of K and then a method of estimating their critical exponents.

Before exposing the techniques used for the numerical study of the model's critical properties, and in order to obtain some idea of the basic characteristics of our model, we shall now discuss earlier predictions concerning the critical behaviour of the lattice version of scale covariant $\lambda\phi^4$ theory.

3. Scale Covariance and Lebowitz violation

As has been stated in the introduction, canonical lattice $\lambda\phi^4$ theory has been rigorously proved to be trivial in d=5 and is almost certainly trivial in d=4 [6]. An essential part of the rigorous proof consists of finding upper and lower bounds for the renormalised coupling g_R. One such bound is obtained by using the Lebowitz inequality [25]. This inequality was proved useful in the study of the IVM, but it is also valid for

the class of systems described by the lattice canonical $\lambda\phi^4$ formulation (B≡0). It is

$$< \sigma_i \sigma_j \sigma_k \sigma_l >_c \leq 0 \qquad (2.19)$$

This implies $g_R \geq 0$ and with minor assumptions [42,43,44], $\gamma \geq 1$ and $\kappa \geq 0$. Frohlich [6] has shown that the connected four point function G_4^c obeys

$$0 \geq G_4^c \geq -a^{d-4} \times \text{constant} \qquad (2.20)$$

from which triviality follows in the $a \to 0$ limit for $d \geq 5$. The left-hand-side inequality of (2.20) can be readily recognised as a consequence of (2.19). If however, the Lebowitz inequality is violated, it immediately follows that (2.20) is no longer true and triviality is not necessarily enforced.

Klauder [29] has given a very simple counterexample for which Lebowitz violation occurs. This is the case of a single site lattice on which we have defined a pseudofree (U_o=0) scale covariant (B≠0) $\lambda\phi^4$ theory. The realy simple argument [41] is as follows :

We define the moments of the single site spin distribution $d\mu(\sigma)$ of (2.10) by

$$\tilde{I}_n(h) = \int d\mu(\sigma)\ \sigma^n \exp(-h\sigma) \qquad (2.21)$$

and the normalised moments by

$$I_n(h) = \tilde{I}_n(h) \; / \; \tilde{I}_o(h) \tag{2.22}$$

Thus, it follows directly that for our single site pseudofree toy model

$$I_{2n}(0) = A^{-n} \; \frac{\Gamma[n+\frac{1}{2}(1-B)]}{\Gamma[\frac{1}{2}(1-B)]} \tag{2.23}$$

But the normalisation condition (2.7), which can now be written as

$$I_2(0) = 1 \tag{2.24}$$

imposes that

$$A = \frac{1}{2} \; (1-B) \tag{2.25}$$

and thus

$$I_{2n} = [\frac{1-B}{2}] \; ^{-n} \; \frac{\Gamma[n+(1-B)/2]}{\Gamma[(1-B)/2]} \tag{2.26}$$

In particular

$$I_4(0) = (1-B)^{-1} \ (3-B) \qquad (2.27)$$

For a single site lattice, the analogue of the connected normalised four-point function is

$$\langle \sigma^4 \rangle_c = I_4(0) - 3 \ I_2(0)^2 = 2 \ B \ (1-B)^{-1} \qquad (2.28)$$

Obviously, this means that for any positive value of B in the allowed interval (0,1), Lebowitz violation occurs. The inequality becomes maximally untrue as $B \to 1-$. This argument, although valid for the simplistic case of an one site lattice, may well be true for the general case of multisite lattices which are the ones of interest. Lebowitz violation would then result for some values of B and subsequently for these regions of B, $\kappa < 0$ is a possibility. Thus, a fine tuning of B can result in κ having positive, negative or zero values. The last case is obviously the one sought. In [29] the possibility of this scenario was demonstrated.

4. Mean Field and Landau approximations

It is important to pay attention to the predictions which can be obtained analytically with the aid of certain approximations. The virtue of such an excercise is twofold : Firstly, it provides a general idea of the coarse characteristics of the model, and gives a first

rough estimate of the values of the critical quantities of interest. Secondly, by exposing the limitations of such methods, it motivates the numerical approach which is the one that will give the more accurate answers. This is the reason we will give a few short proofs of results in full detail.

The first approximation is the well known Mean Field Theory (MFT). The starting point [45] is that each spin is in a local magnetic field h', which consists of the external field h plus the field provided by the neighbouring spins. The average value of a spin in the field h' should be proportional to h' and inversely proportional to the temperature T (Curie Law) :

$$M_1 = \frac{ch'}{T} \tag{2.29}$$

where c is a positive constant (M_1 and h' must not be opposite). Now MFT assumes that the field due to the neighbouring spins is a function of the average of all spins M_1. For small M_1, this field is linear in M_1; thus we have

$$h' = h + aM_1 \tag{2.30}$$

Combining (2.29) and (2.30) we obtain

$$M_1 = \frac{hc}{T-T_c} \qquad (2.31)$$

with

$$T_c \equiv ca \qquad (2.32)$$

Note that (2.31) is the solution to (2.29) and (2.30) provided that $T > T_c$ (otherwise (2.31) states that M_1 points opposite to h). Thus, for $T > T_c$, we have that

$$\chi = \frac{\partial M_1}{\partial h} \propto \frac{1}{T-T_c} \qquad (2.33)$$

which gives the MFT prediction

$$\gamma = 1 \qquad (2.34.a)$$

Other MFT critical exponents are

$$\nu = 0.5 \qquad (2.34.b)$$

and

$$\Delta = 1.5 \qquad (2.34.c)$$

These, with (2.18) give

$$\kappa = d/2 - 2 \qquad (2.34.d)$$

In the canonical theory, MFT is known to be exact for $d > 5$, yielding $\kappa > 0$ and the theory trivial. This is intuitively explained by the argument that the higher the dimensionality of the lattice, the more the nearest neighbours and the better the basic MFT assumption is expected to apply.

Still within the MFT framework, we assert that the average zero-external field magnetisation of a particular site σ (with all other spins "frozen" to their mean value M_1) is

$$\langle \sigma \rangle_{h=o} \overset{MFT}{\equiv} \frac{\int d\mu(\sigma)\ \sigma \exp(K2dM_1\sigma)}{\int d\mu(\sigma)\ \exp(K2dM_1\sigma)} = M_1 \qquad (2.35)$$

Obviously, since $d\mu$ is even in σ, this equation is trivialy satisfied by $M_1=0$, which labels the unmagnetised phase of the system ($K>K_c$). This is the graphical solution of Figure (2.2.a). However, as is depicted in Figure (2.2.b), there may be another, non-zero solution, which for $K < K_c$ labels the magnetised phase. At K_c, provided that the phase transition is second order, the zero and non-zero solutions coincide. This is expressed by (2.35) for $K=K_c$ and moreover, it implies that the zero M_1 derivatives $\left.\frac{\partial}{\partial M_1}\right|_{M_1=0}$ of the left-hand and right-hand

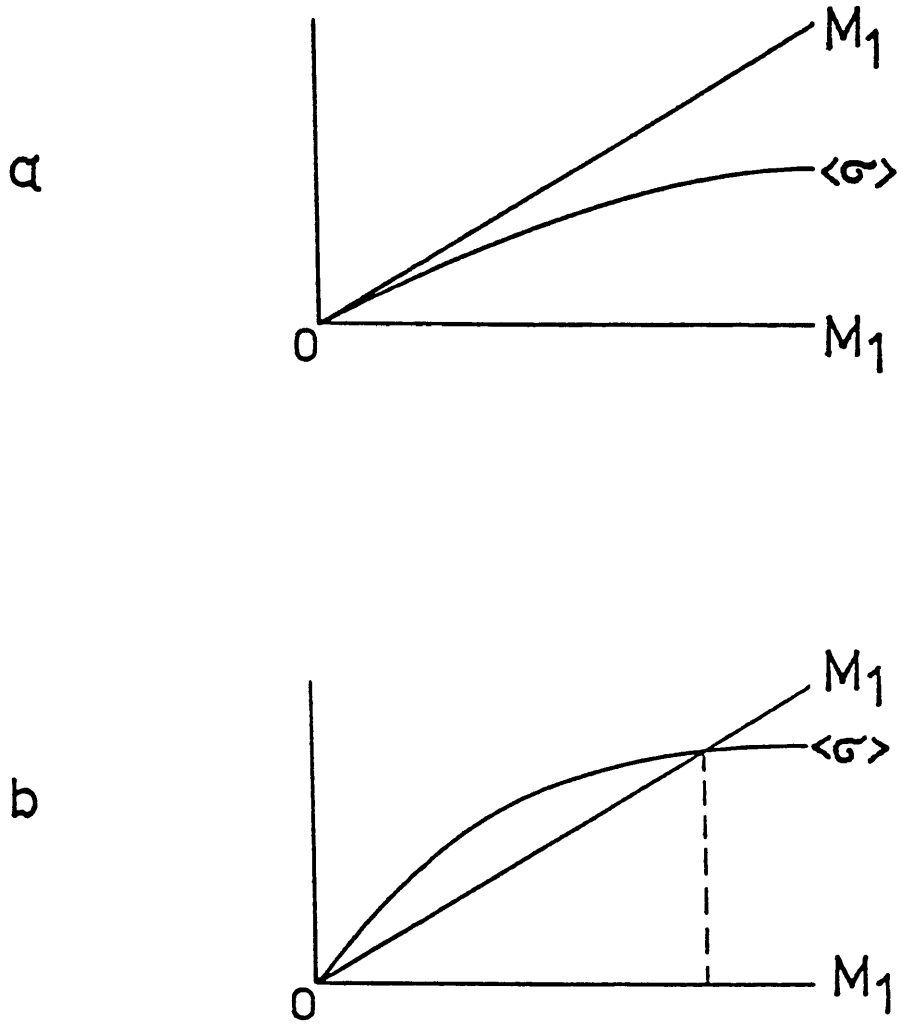


FIG. 2.2 : Graphical solution of equation (2.35) for M_1. In case (a) we have $M_1=0$, while in case (b) we have a non-trivial solution $M_1 \neq 0$. (Reproduced from reference [50])

side of (2.35) remain equal : Thus

$$\frac{\partial}{\partial M_1} M_1 \Big|_{M_1=0} = 1 \qquad (2.36)$$

and, using (2.21) and (2.22)

$$\frac{\partial \langle\sigma\rangle}{\partial M_1} \Big|_{M_1=0} = \frac{K_c 2d\ \tilde{I}_2(0)\ \tilde{I}_0(0) + K_c 2d\ \tilde{I}_1(0)^2}{\tilde{I}_0(0)^2} \Big|_{M_1=0} \qquad (2.37)$$

Using (2.24) and the zero magnetisation property (i.e. $\tilde{I}_o(0)=0$) we have

$$\frac{\partial \langle\sigma\rangle}{\partial M_1} \Big|_{M_1=0} = 2dK_c \qquad (2.38)$$

From (2.36) and (2.38) we obtain the MFT prediction of the critical inverse temperature

$$K_c = 1/2d \qquad (2.39)$$

The reason we have given these proofs in such great detail is to demonstrate the following very important point : Nowhere in these proofs was the scale covariant property (i.e. the presence of B) used. The same value for γ is obtained for any spin theory whatsoever and the same value for K_c results for any continuous spin Ising

model irrespective of the form of the single site spin distribution. The conclusion is therefore that MFT, although a useful tool for a qualitative analysis, is not powerful enough to give accurate predictions. It fails to "see" the "details" of the theory ; and the scaling parameter B is exactly the all important "detail" we are investigating.

The next analytical approach of interest is the Landau semiclassical approximation. According to this theory, given a statistical mechanical system such as the one defined through (2.4) and (2.5), we may define a thermodynamical potential which is a functional of the magnetisation per site M_1 [37]. Expanded in powers of magnetisation it reads :

$$\Gamma[M_1,T] = \Gamma_o(T) + \int d^d x \left(\frac{1}{2} (\nabla M_1)^2 + \frac{1}{2} \alpha(T) M_1^2 + \right.$$

$$\left. \frac{1}{4!} \beta(T) M_1^4 + \frac{1}{6!} \gamma(T) M_1^6 + \ldots \right) \qquad (2.40)$$

where β is given by

$$\beta = \frac{\delta^4 M_1}{\delta M_1^4} \Bigg|_{J=0} = - \chi^{-4} \chi_{(2)} \qquad (2.41)$$

(Note that α, β and γ are coefficients of the power expansion and not critical exponents).

Let us consider the effective potential V_{eff} up to sixth order :

$$V_{eff} = \frac{1}{2}\,\alpha(T)\,M_1^{\,2} + \frac{1}{4!}\,\beta(T)\,M_1^{\,4} + \frac{1}{6!}\,\gamma(T)\,M_1^{\,6} \qquad (2.42)$$

The stability requirement implies that V_{eff} must be bounded below, which in turn imposes that $\gamma > 0$. Then V_{eff} can display different behaviour according to the signs of α and β. As shown in Figure (2.3.a) ,for $\beta > 0$, when $\alpha(T) < 0$ the global minimum is non-zero (magnetised phase) whereas when $\alpha(T) > 0$, the global minimum is zero. Thus, there is a critical temperature T_c (defined through $\alpha(T_c) = 0$) at which the "magnetised" curve deforms into the "unmagnetised" one and its corresponding global non-zero minimum passes smoothly to a zero value. Clearly, the transition is continuous (second order). When, however, $\beta < 0$ the situation is different, as shown in Figure (2.3.b). For $\alpha \leq 0$, we again have a magnetised phase (non-zero global minimum) which persists for certain positive values of α ($\alpha > 0$) provided that $\beta^2 > 4\alpha\gamma$. At a critical temperature T_c (defined through $\beta^2(T_c) = 4\alpha(T_c)\gamma(T_c)$) there coexist two global minima, one zero and one non-zero. As the system is heated further, we get $\beta^2 < 4\alpha\gamma$ and the global minimum is the zero one (unmagnetised phase). The jump from one phase to the other has been discontinuous, and the transition first order.

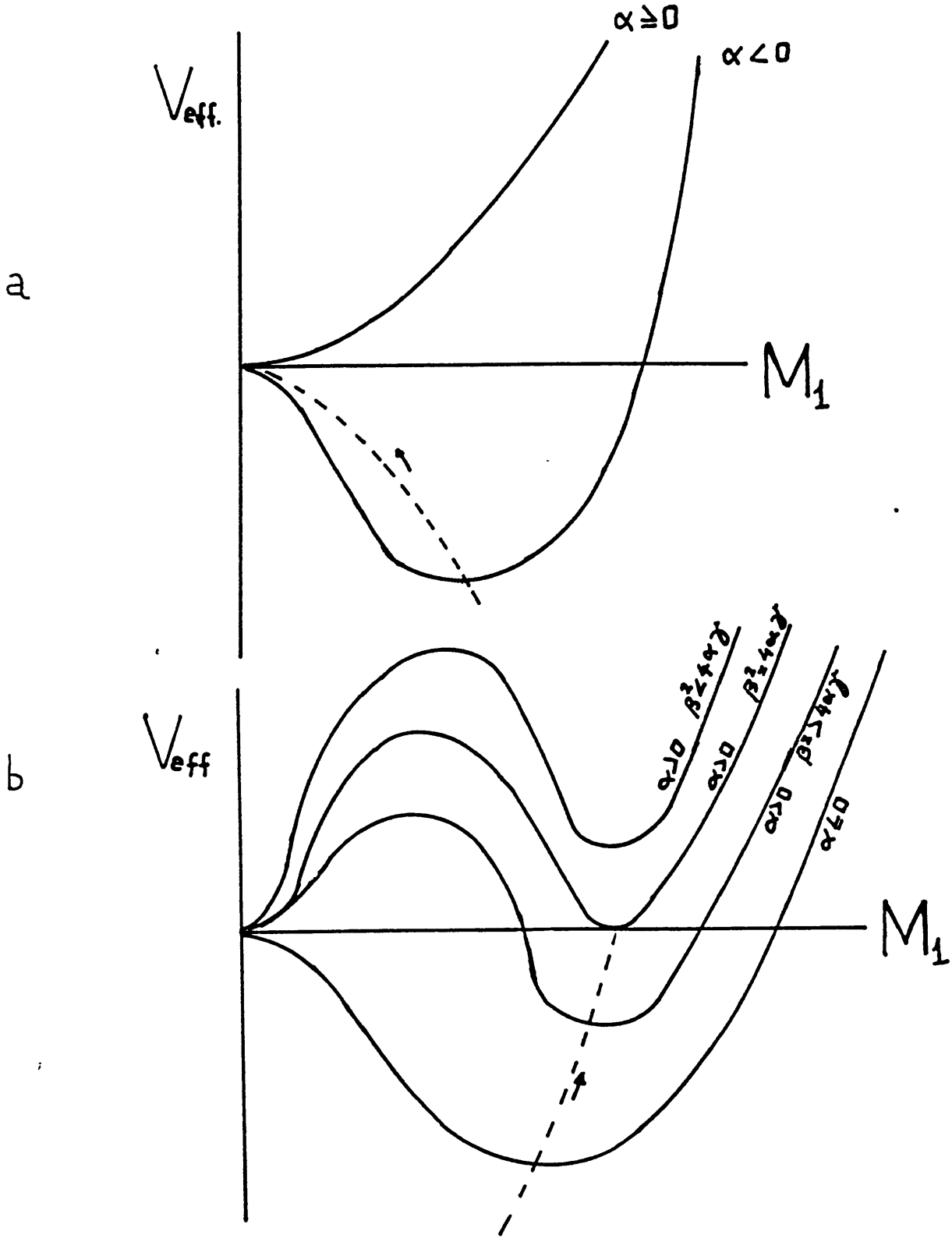


FIG. 2.3 : The effective potential as a function of the magnetisation when (a) $\beta \geq 0$ and (b) $\beta < 0$. The dashed line shows the movement of the global minimum as T (and $\alpha(T)$) is increased.

We have shown that the sign of β (and, through (2.42), that of $\chi_{(2)}$) determines the order of the transition. Therefore, $\chi_{(2)} \leq 0$ implies a second order phase transition and, since it is synonymous to the Lebowitz inequality, it also implies $\kappa \geq 0$. Conversely, $\chi_{(2)} > 0$ implies a first order phase transition, a violation of Lebowitz inequality, and thus the possibility of negative κ. This situation is illustrated in Figure (2.4).

From it, we derive the final prediction of the Landau semiclassical approximation : There is a region in the B-U_o plane for which the transition is second order, and the Lebowitz inequality is valid; i.e. $\kappa \geq 0$. This is separated by a line of tricritical points from a region of first order transistions in which Lebowitz is violated; i.e. κ is permitted to have negative values. If we assume smooth variations and changes of sign for κ with B and U_o, there is a line in the B - U_o plane for which $\kappa = 0$. This line must be entirely in the discontinuous transition region (otherwise, $\kappa < 0$ values would be allowed in places where Lebowitz is valid) but is permitted to touch the tricritical line. Thus, Landau type arguments suggest that although the possibility of a non trivial lattice theory which has a "tricritical-boundary-type" continuum limit cannot be in principle excluded, trying to locate it on a single point of the B - U_o plane with numerical techniques appears unrealistic. However, the Landau theory is just a

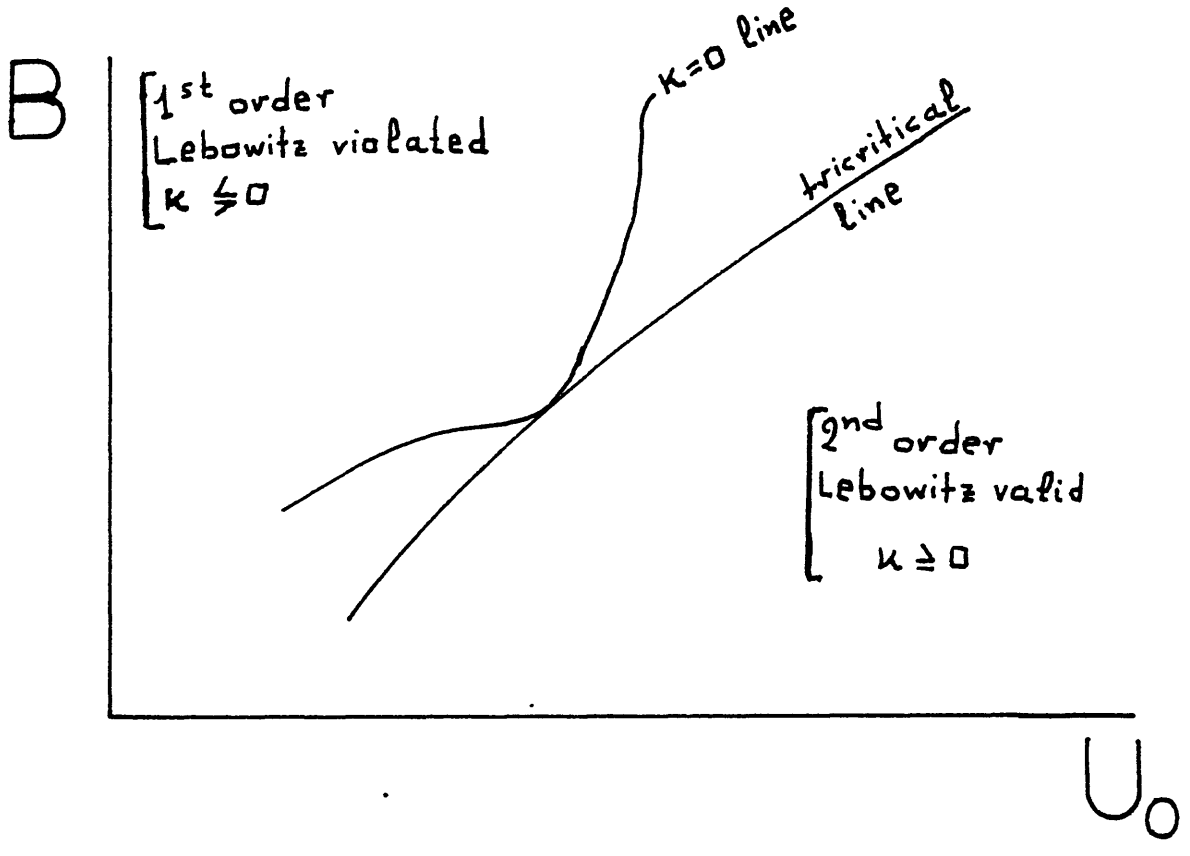


FIG.2.4 : Schematic representation on the $B-U_0$ plane of the predictions of the Landau approximation.

semiclassical approximation and the full quantum effects can alter the picture.

The Landau approximation has been useful in two ways. Firstly, it has signaled the possibility of a first order phase transition ; a case which has been neglected in earlier analyses [29,41]. Secondly, it again gave results which are independent of the scaling parameter B. Consequently, if we want to see the influence of B, we must turn our attention away from approximation techniques. The natural alternative is series expansions.

5. Early results from series analysis

Having experienced the limitations of approximation techniques, we now turn our attention to series expansions. Since series expansions and series extrapolations are amongst the main techniques that this thesis relies on, we shall not refer to them extensively in this section ; they will be properly presented in the next chapter. For the moment we shall only state that the thermodynamical quantities defined by (2.12) and (2.13) can be evaluated as series in powers of the inverse temperature K with coefficients which depend on the model's parameters B and U_o. One can then use Pade approximants (which will also be presented in the next chapter) to evaluate the critical exponents.

Klauder [29] has used these techniques in order to

analyse the pseudofree (U_o=0) scale covariant (B≠0) theory in four dimensions. His results for κ and for different values of B are plotted in Figure (2.5). The encouraging result from this plot is that, like for the example of the one site lattice theory, there seems to be a value of B in the interval (0,1) for which κ can be zero. Thus, as in the large N analysis of Rivers [35] and Gent [36], a fine tuning of B can result in a pseudofree theory which is non-trivial and distinct from the trivial (Gaussian) free theory. The alarming aspect of this result, however, is a surprisingly large variation of γ, ν, Δ and κ with B. Such a violation of universality is a very unwelcome result and requires further investigation. At this stage, we will only state that since it is only assumed (and not proved) that the phase transition is second order, certain of these results, which are based on this assumption, may not make sence. Also, neglecting confluent singularities may be another cause of this anomaly. The question of universality will be examined in the next Section and at latter stages of the thesis. In any case, it is clear that Klauder's work indicates a possible way out of triviality but his analysis is only at a preliminary level. In what follows we shall adopt his approach for the fully interacting theory (U_o≠0) and supplement it with an examination of the order of the phase transition. We shall see that this will alter the final conclusions.

More recently, Rivers has examined the behaviour of

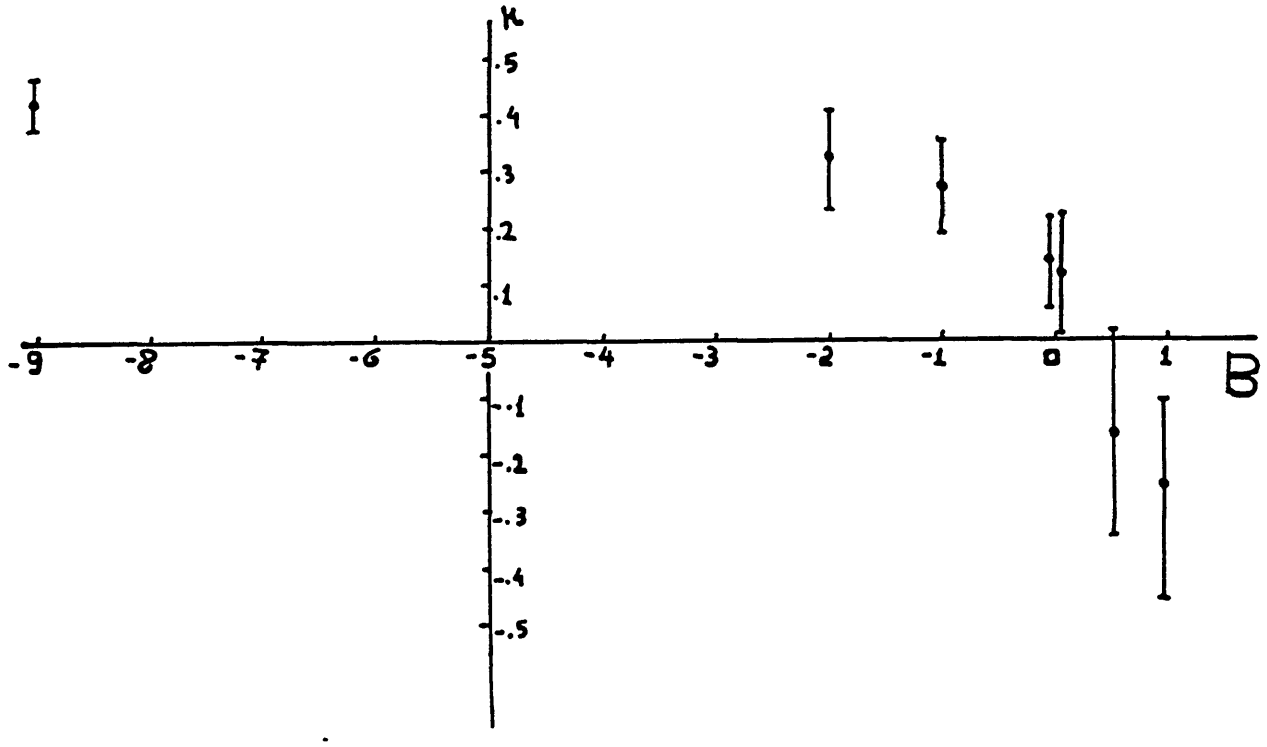


FIG. 2.5 : Variation of κ with B for $U_0 = 0$ and A=0.5. The results were obtained by using series expansions and Pade approximants.

the coefficients of the high themperature series in the limit $B \to 1^-$ (in which the theory becomes scale invariant) and for $U_o = 0$ (pseudofree case) [41]. He found that in this limit the series coefficients depend very simply on the moments of the spin distribution. Using ratio methods to analyse the series, the critical exponents of the scale invariant theory turn out to be

$$\gamma = 0.5 \qquad (2.43.a)$$

$$\Delta = 0.5 \qquad (2.43.b)$$

$$\nu = 0 \qquad (2.43.c)$$

whence

$$\kappa = -0.5 \qquad (2.43.d)$$

independent of dimension. This means that the pseudofree scale invariant theory does not exist in any dimensions. However, Rivers points out that even a superficial examination of the behaviour of K_c reveals that the pseudofree scale covariant model in the $B \to 1-$ limit (as examined numerically in [29]) has properties which are disconnected from those of the scale invariant model (for which $B \equiv 1-\varepsilon$; ε small). The two limiting proceedures are not equivalent. Thus, the properties of the scale invariant pseudofree theory can be of limited use to an

examination of the full ($B \neq 0$, $U_o \neq 0$) theory.

From the discussion of the last two sections it is apparent that the approximation methods have failed to enlighten the situation. The only encouraging results come from the numerical analysis of Klauder [29]. It is therefore evident that one must attempt to clarify the situation in this direction. The numerical analysis which is exposed in subsequent chapters is a non-trivial generalisation and extension of the numerical analysis to its limits. We have, however, proceeded in the spirit of this early work [29].

6. A comment on universality

In the next chapter, we shall explicitly calculate numerically the values of the critical temperature and critical exponents of the model. Given a pair of values for the bare parameters B and U_o, we shall evaluate the inverse temperature K_c for which the model has an (assumed) second order phase transition and the critical exponents near K_c. However, even if the assumption concerning the order of the transition is correct, we are not guaranteed a continuum field theory at K_c. This is because a second order phase transition is a necessary but not sufficient condition for the continuum field theory to exist ; the continuum theory lives only at the phase transition point of the phase diagram for which the renormalised mass m_R (the two point Green' s function)

has a fixed physical value. As we will perform our measurements in the bare parameter space (B-U_o) without fixing m_R, the analysis that will follow may appear dubious at first sight.

This is not so ; since we will not be measuring the coupling constant g_R but only the corresponding critical exponent κ, we do not need to consider renormalisation aspects of the problem carefully. The information we are seeking concerns primarily only the sign of κ. Thus, two alternatives seem plausible : (a) The critical exponents turn out to be universal. They do not vary with B and U_o. This view is supported by most results obtained for more conventional spin models. It has recently been stated that the principle of universality may not be valid in its 'stronger' sense in the $\lambda\phi^4$case [46]. It is possible that continuous spin theories are characterised by a 'weaker' universality ; i.e. there are different regions of their parameter space, each labelled by a different shape of the single site spin distribution, in which the critical exponents are universal but different from those in other regions. This point will be treated in greater detail in Chapter V. (b) The critical exponents are smooth functions of B and U_o. This sounds intuitively plausible and is supported by the numerical data of Klauder [29] but is a very unwelcome situation as it contradicts the generally accepted principles of Statistical Mechanics.

For the moment, we shall not attempt to clarify which of the two possibilities is true. This will be postponed intil Chapter V. In either case, however, careful renormalisation becomes redundant : By performing measurements over a large number of points in the $B-U_o$ plane (the real parameter space) we may establish the behaviour of the critical exponents at all critical points. We will be able to deduce their behaviour at the theory's continuum limit, irrespective of whether this behaviour turns out to be universal or smoothly varying.

CHAPTER III

HIGH TEMPERATURE ANALYSIS

1. High temperature expansions

We shall now introduce briefly the way to obtain high temperature series expansions (i.e. expansions in powers of K) for the thermodynamical quantities of interest. We have used the results of Kincaid et. al. [47] who rely on the method of Wortis [48] to obtain their series. As the general methodology is described in great detail in [48] and its application to any continuous spin Ising model is fully given in [47], we shall only give a brief outline of the main idea, referring the reader to the above referenes for details and proofs. A fuller exposition of the techniques and the results of this Chapter can also be found in [49].

Having defined the moments I_n and $\tilde{I}_n$ of the single site spin distribution $d\mu(\sigma)$ (see equations (2.21) and (2.22)), we recall that the magnetisation per site k is given by

$$M_1(k) = \langle \sigma_k \rangle = Z[h]^{-1} \int [\prod_i d\mu(\sigma_i)] \, \sigma_k \exp(-S[\sigma]) \quad (3.1)$$

It is easy to verify that

$$M_1(k) = \frac{1}{Z}\frac{\delta Z}{\delta h_k} \qquad (3.2)$$

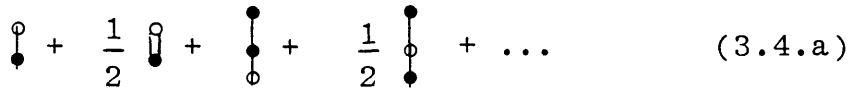
We observe that all the quantities of interest are expressible as functional derivatives of $M_1(k)$:

$$\chi = \sum_k \frac{\delta M_1(0)}{\delta h_k} \qquad (3.3.a)$$

$$\chi_{(2)} = \sum_{klm} \cdot \frac{\delta^3 M_1(0)}{\delta h_k \delta h_l \delta h_m} \qquad (3.3.b)$$

$$\mu_2 = \sum_k \frac{k_\mu k_\mu}{a^2} \frac{\delta M_1(0)}{\delta h_k} \qquad (3.3.c)$$

We can now develop (in the limit of low K) the exponential of eqn. (3.1) as a series expansion in powers of K and thus obtain the magnetisation as a power series in K. This expansion, systematised in terms of lattice graphs, can be carried out by using a complete set of diagrammatic topological and algebraic rules [48]. In order to give a flavour of the Wortis method, we quote just one result. The diagramatic expansion for the magnetisation per site is given by the sum of all topologically distinct 1-rooted connected graphs according to Rule 2 of Wortis. This expansion, to order K^2 looks like

$M_1(k) =$  (3.4.a)

which, according to Rule 2 of Wortis corresponds to the algebraic expression

$$M_1(k) = M_1^o(k) + \sum_l M_2^o(k)\, K(k,l)\, M_1^o(l) +$$

$$\frac{1}{2} \sum_l M_3^o(k)\, K(k,l)^2\, M_2^o(l) +$$

$$\sum_{l,m} M_2^o(k)\, K(k,l)\, M_2^o(l)\, K(l,m)\, M_1^o(m) +$$

$$\frac{1}{2} \sum_{l,m} M_3^o(k)\, K(k,l)\, M_1^o(l)\, K(k,m)\, M_1^o(m) + \ldots \qquad (3.4.b)$$

where

$$K(i,j) \equiv K\, \delta_{j,i+\underline{\mu}} \qquad \forall\, \underline{\mu} \qquad (3.5)$$

and

$$M_n^o(k) \equiv M_n^o(h_k) \equiv \frac{d^n}{dh_k^n} \ln\left(\tilde{I}_o(h_k)\right) \qquad (3.6)$$

One can refine such diagramatic techniques to a

great extent ; Wortis's 'linked cluster expansion' artillery consists of 19 diagramatic rules. Essentially, these rules systematise the following three fundamental procedures which are necessary for carying out the expansion. They are :

(i) enumeration of the contributing graphs

(ii) calculation of the contribution of each graph

(iii) addition

Step (ii) usually consists of two parts : (a) a factor that depends on the graph's topology, called weight and (b) the graph's multiplicity which is determined by the number of different ways it can be embeded in the underlying lattice.

Utilising the method in order to carry out the calculation to a sufficiently high order is no easy task. Typically, the first few coefficients are trivial and no special methodology is necessary for their calculation. However, in higher orders the bookkeeping is extremely involved. Kincaid et. al. [47] have listed the necessary graphs, their symmetry factors and free multiplicities for the calculation of the series for M_1, χ, $\chi_{(2)}$ and μ_2 to tenth order in K and for eight lattices (linear chain, square, triangular, cubic, body-centered cubic, face centered cubic, hypercubic and hyper-body-centerd cubic). The outcome is that $M_1(h)$ and consequently χ, $\chi_{(2)}$ and μ_2 can be evaluated as a power series of the form

$$F(K) = \sum_{k=0}^{\infty} f_n K^n \qquad (3.7)$$

where the coefficients f_n are polynomials of certain even order normalised moments $I_{2m}(h)$ as defined in (2.22). Note that the coefficients f_n only depend on certain moments I_{2m} irrespective of the single site spin distribution through which these moments are defined. This means that the results of Kincaid et. al. can be used with any single site spin distribution, including our scale covariant $d\mu(\sigma)$.

We have utilised their results as follows : Recall that the normalisation condition (2.24) can be solved numerically to give A, for any pair of (B, U_o) values. Having obtained A, the computer was then used to generate the even moments, up to $\tilde{I}_{14}(0)$, which are necessary for the high temperature expansions to tenth order in K. This was simply done by performing the integration of (2.21) numerically using the NaG 8 Fortran Library . From these moments, and their coefficients tabulated by Kincaid et. al., the computer was then used to generate the actual high temperature series to tenth order in K for χ, $\chi_{(2)}$, μ_2. These being known, we used (2.13) to generate the high temperature expansions of ξ and g_R to the same order.

2. Pade Approximants

We have outlined how, by using the method of high temperature analysis certain physical quantities of interest (collectively denoted here by F(K)) can be represented by p- order power series of the form

$$F(K) = \sum_{n=0}^{p} f_n K^n + O(K^{p+1}) \qquad (3.8)$$

(in our case we saw that p = 10). We shall assume that the $O(K^{p+1})$ terms do not contribute significantly and shall neglect them from now on. This can be dangerous (e.g. for conventional $\lambda\phi^4$ in d = 3, p = 10 does not resolve the question of triviality since it gives the result $\kappa=0.028 \pm 0.003$ [14]) but we can only adhere to the present day available accuracy which has been sufficient for the d=4 conventional $\lambda\phi^4$ theory for which $\kappa=0.30 \pm 0.04$ [14].

Since we assume that in the critical region of interest the behaviour of F(K) is described by

$$F(K) = f(K)\ (K-K_c)^{\varepsilon} \qquad (3.9)$$

(f(K) analytic in K_c), we want to utilise the series approximation of (3.8) in order to extract estimates for K_c and ε. The standard method is to use Pade approximants. This method is meant to be a good approximation of functions F(K) in their circle of meromorphy except for those regions of K where they

display branch point singularities. Unfortunately, eqn. (3.9) suggests that the critical region has such a singularity at K_c. To circumvent this problem, we used a variant of the Pade analysis known as D-log Pade which we now describe : We first observe that

$$\frac{d}{dK} \ln F(K) = \frac{dF(K)}{dK} F(K)^{-1} \qquad (3.10)$$

Since F(K) is represneted by a p-order power series in K, $\frac{d}{dK}\ln F(K)$ is also known as a p-1 order power series by virtue of (3.10). Thus, given the f_n's of (3.8) we can uniquely determine the c_n's of the expansion

$$\frac{d}{dK} \ln F(K) = \sum_{n=0}^{p-1} c_n K^n \qquad (3.11)$$

From (3.9) it is obvious that as $K \to K_c^-$,

$$\frac{d}{dK} \ln F(K) = \frac{\varepsilon}{K-K_c} + \frac{d}{dK} \ln f(K) \qquad (3.12)$$

This has a simple pole at $K = K_c$ with residue ε, so we expect it to be well approximated by the Pade approximants, which we now define.

Given the series of eqn. (3.11) we define its [L/M] Pade approximant as the following ratio of polynomials

$$[L/M](K) \equiv \frac{R_L(K)}{Q_M(K)} \equiv \frac{\sum_{l=0}^{L} r_l K^l}{\sum_{m=0}^{M} q_m K^m} \qquad (3.13)$$

with $q_0 = 1$. Equating the right hand sides of (3.11) and (3.13) we get

$$\Sigma c_n K^n \simeq [L/M](K) \equiv \frac{R_L(K)}{Q_M(K)} \qquad (3.14)$$

and provided that $L+M < p-1$, the coefficients r_l, q_m are uniquely defined in terms of the coefficients c_n [49,51].

The claim is that the approximants [L/M], thus obtained, converge to F(K) as their order increases. This is not generally true, although there are theorems that guarantee that, for certain special cases of functions F(K), the approximants converge to F(K) [52]. Our functions F(K) do not have any properties that would theoretically guarantee convergence of the approximants. It is true, however, that the maximum region of convergence of sequences of Pade approximants exceeds that of a Taylor series. If F(K) has p poles in its circle of meromorphy, the circle of convergence of a Taylor series extends only up to the pole which is closest to the origin. The [L/M] sequance of Pade approximants, however, converges uniformly to F(K) as L →

∞ everywhere inside the circle of meromorphy, except at the neighbourhoods of the p poles [53,54]. In practice [54], convergence is still satisfactory in the vicinity of the poles near the origin for $M < p$. These results are justified by the fact that the poles of F(K) can be represented naturally by Pade approximants since they are defined to have a pole structure (cf. equation (3.13)). Combining theory and experience from numerical experiments we can expect our series to be sufficiently well approximated by Pade approximants as obtained from (3.13).

The M zeroes of the polynomial $Q_M(K)$ in the denominator give the possible values of K_c, while the polynomial $R_L(K)$ evaluated at K_c gives values for ε. The relevant pole out of the M candidates is picked by requiring consistency between different order Pade approximats : the pole at K_c must remain stationary while other poles will move around between different order approximants.

This process was carried out by computer. From the f_n's of the F(K) series, the c_n's of the D-log series were calculated. The [L/M] approximants to this series were then calculated for $1 \leq L,M \leq 5$ and their poles and residues found numerically. This gave possible values of K_c and ε.

3. Practical aspects and consistency of Pade approximants

We insist that our series are such that Pade approximants are not theoretically guaranteed to work. Trouble can arise; for instance increasing the order of the approximant does not necessarily improve the accuracy close to the singularity of interest. Another problem is the appearance of spurious poles and almost coincident zeros in regions close to the origin where F(K) is analytic. Despite all this, practice has shown that in many occasions [51,55] the diagonal [L/L] and near diagonal [L+j/L] approximants give good results. Nevertheless, the lack of theoretical justification becomes apparent in cases where the approximants fail to give meaningful answers for no obvious reason. To extract reasonable estimates, we have used three different methods of Pade-approximating the series of interest. In all cases, at least one method will yield approximants which provide self consistent estimates for K_c and ε. Occasionally, two or all the methods work well, providing us with consistency checks. The three methods we used are presently described.

Method 1: The D-log Pade approximants of the threee high temperature series of χ, $\chi_{(2)}$ and μ_2 gave three estimates of K_c and a single estimate for each of γ, Δ and ν. The values and apparent statistical errors of these estimates were obtained by calculating the means and standard deviations of the results of the [L/M] approximants for $3 \leq L,M \leq 5$ (i.e. the near diagonal high order approximants). A weighted mean was calculated from the

three estimates of K_c and a value for the critical exponent κ was obtained from γ, ν and Δ using eqn. (2.18). The weakness of this method is that although the three exponents γ, ν and Δ have reasonable individual errors, these sometimes add up to give rather imprecise values of κ with big errors. As an example, we present typical Pade tables obtained from this method for B=0.8 and U_o=0.1 (Table (3.1.a, b, c)). The final results are collected in Table (3.1.e).

Method 2: A series for g_R was obtained from the χ, $\chi_{(2)}$ and μ_2 series using equations (2.13.a,b). This was then analysed using D-log Pade approximants to give a further estimate of K_c and a direct estimate of κ. The weakness now is that in our search for non-triviality we are primarily interested in locating values of B and U_o for which $\kappa = 0$. If this is the case, the D- log Pade approximant of the g_R series will be expected to simulate a zero residue at K_c (see eqn. (3.12)). So it either collapses by modelling 'irrelevant' singularities or, at best, it models non leading singularities. Thus, this method can be an improvement on the errors of κ compared to those from the previous method, but only in cases where $\kappa \neq 0$. As an example, we provide the Pade table obtained from this method (Table (3.1.d)) for the same B and U_o points as in the example of the previous method. The comparison of the results from both methods is given in Table (3.1.e). In those cases where Method 1 provides us with values of κ which are compatible with zero, the

(a)

M \ L	3	4	5
3	.12102 -1.01407	.12104 -1.01474	.12083 -1.00684
4	.12104 -1.01479	.12101 -1.01377	.12136 -1.02455
5	.12106 -1.01544	.12169 -1.03662	

(b)

M \ L	3	4	5
3	.12005 -3.29304	.11974 -3.23574	.11973 -3.23398
4	.11966 -3.22128	.12005 -3.23574	.11919 -3.16179
5	.12053 -3.39906	.11822 -3.05196	

(c)

M \ L	3	4	5
3	.12104 -2.02829	.12113 -2.02735	.12079 -1.98800
4	.12113 -2.02719	.12097 -2.02450	.12113 -2.02735
5	.12069 -1.95299	.12113 -2.02719	

(d)

M \ L	3	4	5
3	.12639 .77762	.12846 .86603	.12821 .85629
4	.12882 .88285	.12639 .77761	***
5	.12884 .88371	***	

(e)

	METHOD 1	METHOD 2
K_c	.12100(9)	.128 (1)
γ	1.018 (8)	------
Δ	1.11 (5)	------
ν	.50 (1)	------
κ	.8 (1)	.84 (5)

TABLE 3.1 : (a) The L/M Pade table of the χ series at B=0.8 and U_0=0.1. The top number is the position of the pole (K_c) and the bottom number is the associated residue (critical exponent ϵ).
(b) same as (a) for the $\chi_{(2)}$ series.
(c) same as (a) for the μ_2 series.
(d) same as (a) for the g_R series. The asterisks indicate that no pole can be chosen consistently.
(e) Final results for K_c and the critical exponents as obtained from Tables (a) to (c) (Method 1) and Table (d) (Method 2). Figures in brackets indicate the statistical errors between different order Pade approximants.

simultaneous collapse of Method 2 has been used as corroborative evidence (see Table (3.2)).

Method 3: If $\ell n \frac{dF}{dK}$ has the critical behaviour of eqn. (3.13), then we expect that

$$(K-K_c) \frac{d}{dk} \ell n\ F(K) = \varepsilon + 0\ (K-K_c) \qquad (3.15)$$

When F(K) is the series for g_R (and thus, ε is the critical exponent κ) we can use a good estimate of K_c as evaluated from Method 1 and obtain the left hand side of the above equation as a power series. The Pade approximant of this will then be evaluated at K_c to give a better estimate for κ [54]. Just like in the case of the previous method, this method is unreliable when κ=0. As our input value for K_c has also been obtained with the Pade method (and so, it is not an independent estimate) we did not use this method widely.

We again wish to stress that eqn. (3.9) describes only the dominant power law behaviour near the critical region. The possibility of the existence of less dominant confluent power and logarithmic singularities cannot be excluded. Their presence is in principle a source of small systematic errors in the calculation of critical exponents and their detection is not staightforward. The systematic errors they introduce are indeed very small (for example, in a study of 2-dimensional canonical $\lambda\phi^4$, neglecting confluent

	METHOD 1					METHOD 2	
B	K_c	γ	ν	Δ	κ	K_c	κ
.05	.12415(2)	.9951(1)	.496 (2)	1.37(6)	.2(1)	.128 (3)	.16(3)
.10	.12284(2)	.987(6)	.490(4)	1.37(5)	.2(1)	.140 (3)	.21(3)
.35	.1140 (2)	.927(7)	.44 (1)	1.27(1)	.15(6)	.158 (1)	.214(6)
.45	.1088 (3)	.89 (1)	.40 (2)	1.21(2)	.06(9)	***	---
.85	.0673 (6)	.61 (5)	.13 (8)	.73(3)	-.3 (3)	.0572(1)	-.080(1)

TABLE 3.2 : Same as Table (3.1.e) for U =0.001 and various B values. The asterisks indicate that no pole could be chosen consistently from the Pade table at this B value.

singularities results in $\gamma = 1.92 \pm 0.06$; to be compared to $\gamma = 1.996 \pm 0.02$ when they are taken into account [46]). The conventional practice has been to neglect their influence when using Pade approximants and treat the calculation as a "zeroth order" estimation of the critical exponents. This approach has been used both by Baker and Kincaid [15] for studying conventional $\lambda\phi^4$ ($B=0$, $U_o \neq 0$) and by Klauder [29] for the pseudofree theory ($B \neq 0$, $U_o = 0$). In this work, we follow the spirit of Baker, Kincaid and Klauder and adopt their approach to the study of the more general scale covariant theory ($B \neq 0, U_o \neq 0$). In Section 4, we present our "zeroth order" estimates for the values of γ, ν, Δ and κ. An analysis which takes the subdominant critical behaviour into account will be presented in Chapter V.

4. Results from the series analysis

Having discussed so far the methods used, we now present our results, which concern the behaviour of the critical exponent κ in the d=4 case. We have already mentioned that Klauder had already done so for the pseudofree case ($U_o = 0$) and for A = 0.5 (reference [29] and Figure (2.5)). He found evidence for the existence of a non-trivial pseudofree theory for some value of B in the interval (0,1). Our results are in agreement with his, but we have extended the analysis to the full interacting theory ($U_o \neq 0$).

It was found that as the scaling parameter B is increased from zero to one at fixed U_o, the critical exponent κ remains positive for most values of B and U_o (see Figure (3.1)). For U_o sufficiently small, and B sufficiently close to one, however, the critical exponent κ becomes negative. This behaviour is fully illustrated in Figure (3.2.a, b, c, d, e) for the typical case of U_o = 0.001 and for $B \varepsilon (0,1)$. If we assume that κ is a continuous function of B and U_o, it follows that there is a region in the B-U_o plane in which $\kappa \leq 0$. We recall that $\kappa = 0$ is the necessary condition for non triviality; thus a non- trivial solution can only exist at a specific tuned value (or set of values) of B as a function of U_o.

Several comments are appropriate here : First, at points in the B-U_o plane where κ is very close to zero, the consistency checks mentioned above yield poor results due to the failure of Methods 2 and 3 as discussed previously. Away from this region, the results of the three methods were reasonably consistent. Second, we note that as $B \to 1^-$, the coefficients of the high temperature series diverge as a result of the divergence of the moments $\tilde{I}_n$ (see eqn. (2.21)). For this reason, we expect the series to be invalid in this limit, and hence the results of our analysis to be less reliable in this region. Thirdly, we have performed some measurements for $B < 0$ where we find $\kappa > 0$. There are strong indications that for $B < 0$ the model is in the same universality

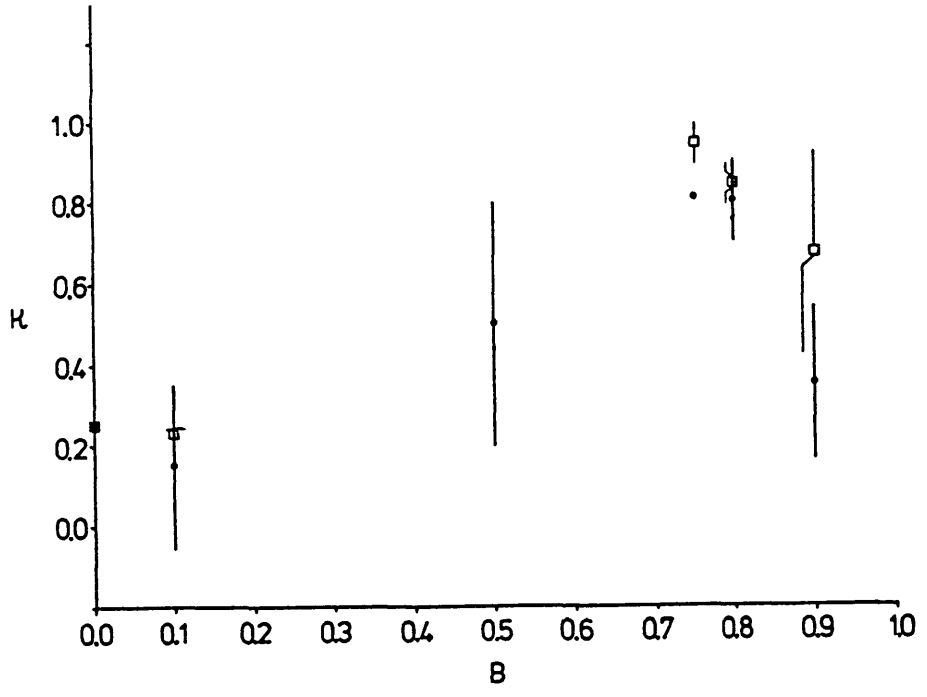


FIG. 3.1 : The variation of κ with B for U_o =0.1 Dots indicate results obtained from Method 1; squares indicate results obtained from Method 2.

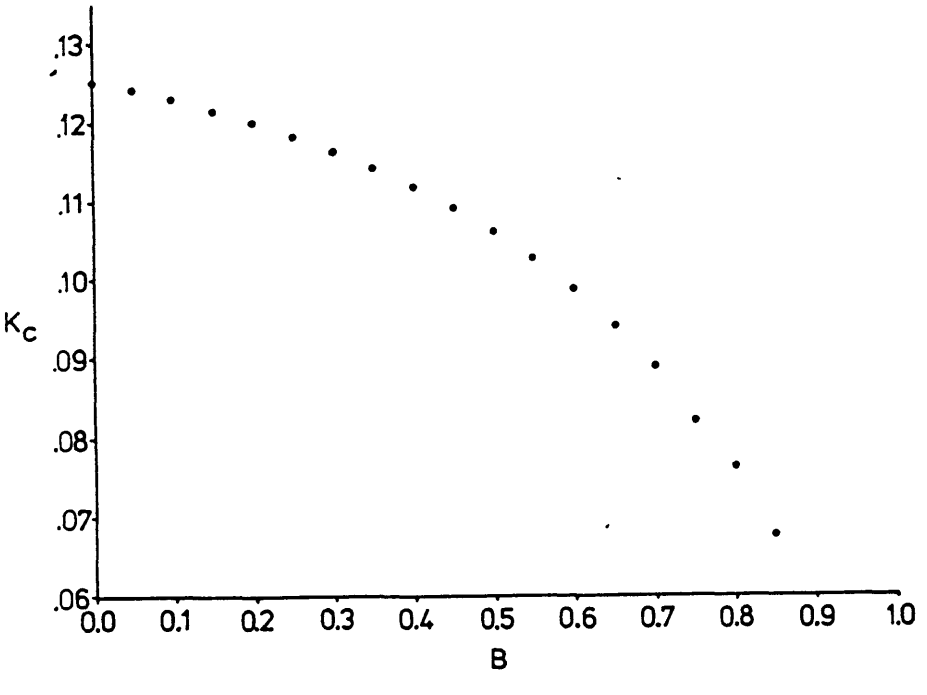


FIG. 3.2 (a) : The variation of K_c with B for U_o=0.001. The statistical errors are too small to be plotted.

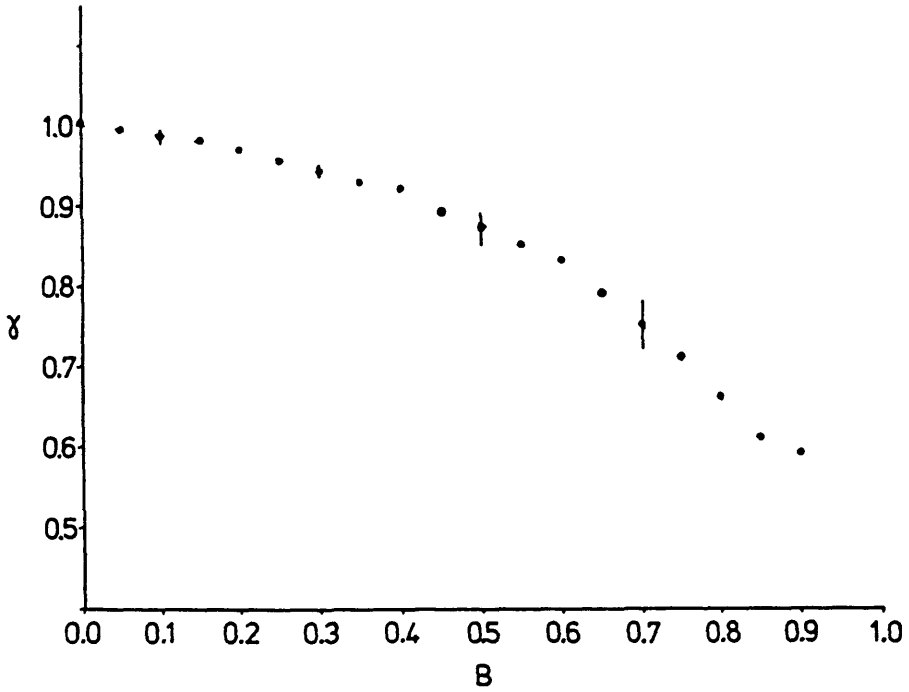


FIG. 3.2 (b) : The variation of γ with B for U_o=0.001.

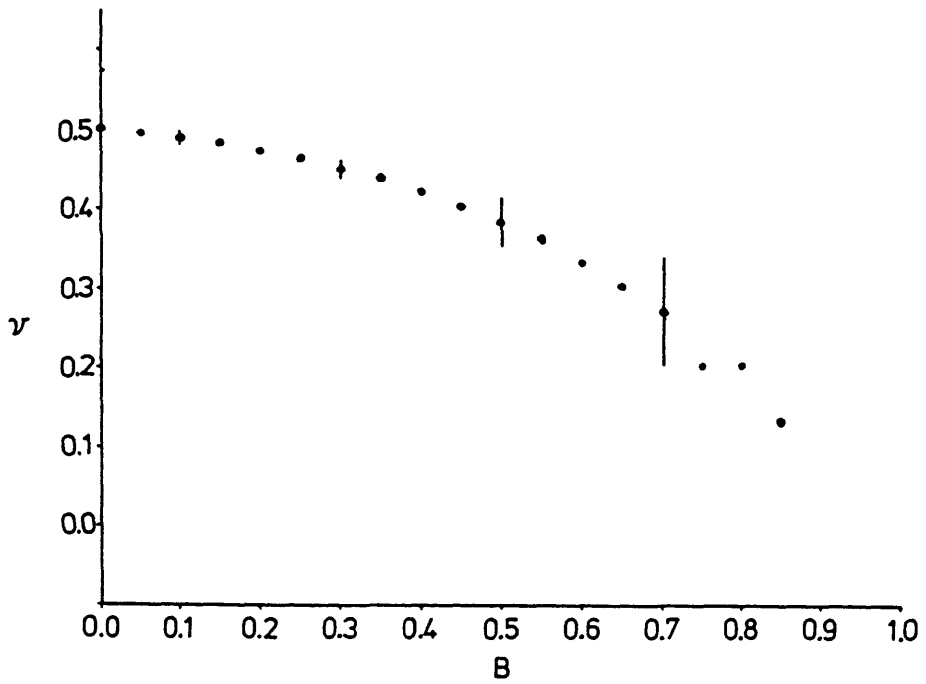


FIG. 3.2 (c) : Same as Figure 3.2 (b) for ν.

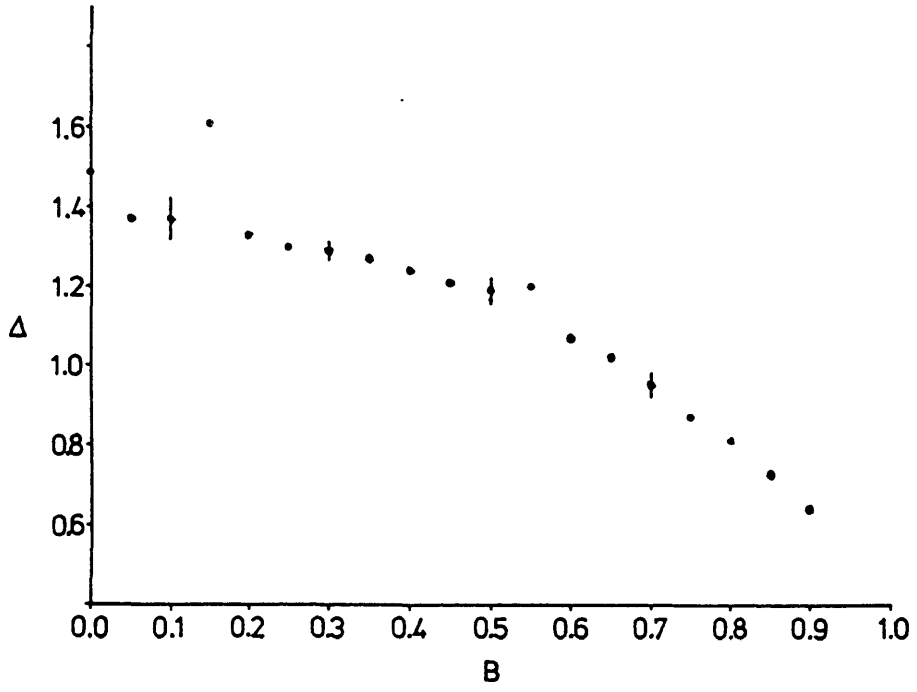


FIG. 3.2 (d) : Same as Figure 3.2 (b) for Δ.

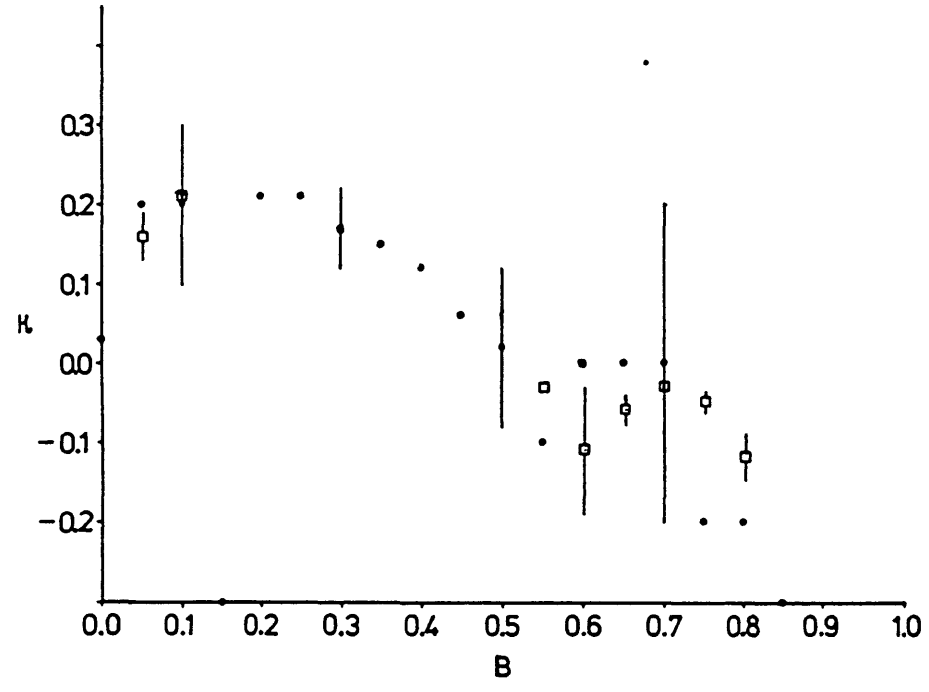


FIG. 3.2 (e) : Same as Figure 3.1 for U_o=0.001.

class as the Ising model [37,56], which has the same fixed point with the ("almost certainly") trivial canonical $\lambda\phi^4$ field theory[12]. As our results indicate that the theory is trivial in this region, we have concentrared our attention on the interval $0 < B < 1$.

One final point ought to be made again. Our data, just like Klauder's [29], indicates very strongly a smooth non-universal behaviour of K_c with B and U_o. This may be due to the fact that our Pade approximants, although they have worked with surprising consistency, may have systematic errors. The source of these errors may be any of the following : (a) finiteness of the series expansion ; (b) neglect of confluent and logarithmic singularities ; (c) a first order phase transition may be setting in exactly in the region of the $B - U_o$ plane for which the critical exponents display the wildest variation with the bare parameters. This latter source of errors can be a serious one, since Pade approximants are based on the conjecture of a second order phase transition. We shall examine this possibility in the Chapter IV. In Chapter V we shall investigate whether a confluent singularity behaviour influences the results. There is nothing that can be done to remedy the problem of the finiteness of our series apart from increasing their order so that higher approximants may be constructed. Such an extensive project is beyond the scope of this work.

In Figure (3.3), we plot the points of the $B-U_o$

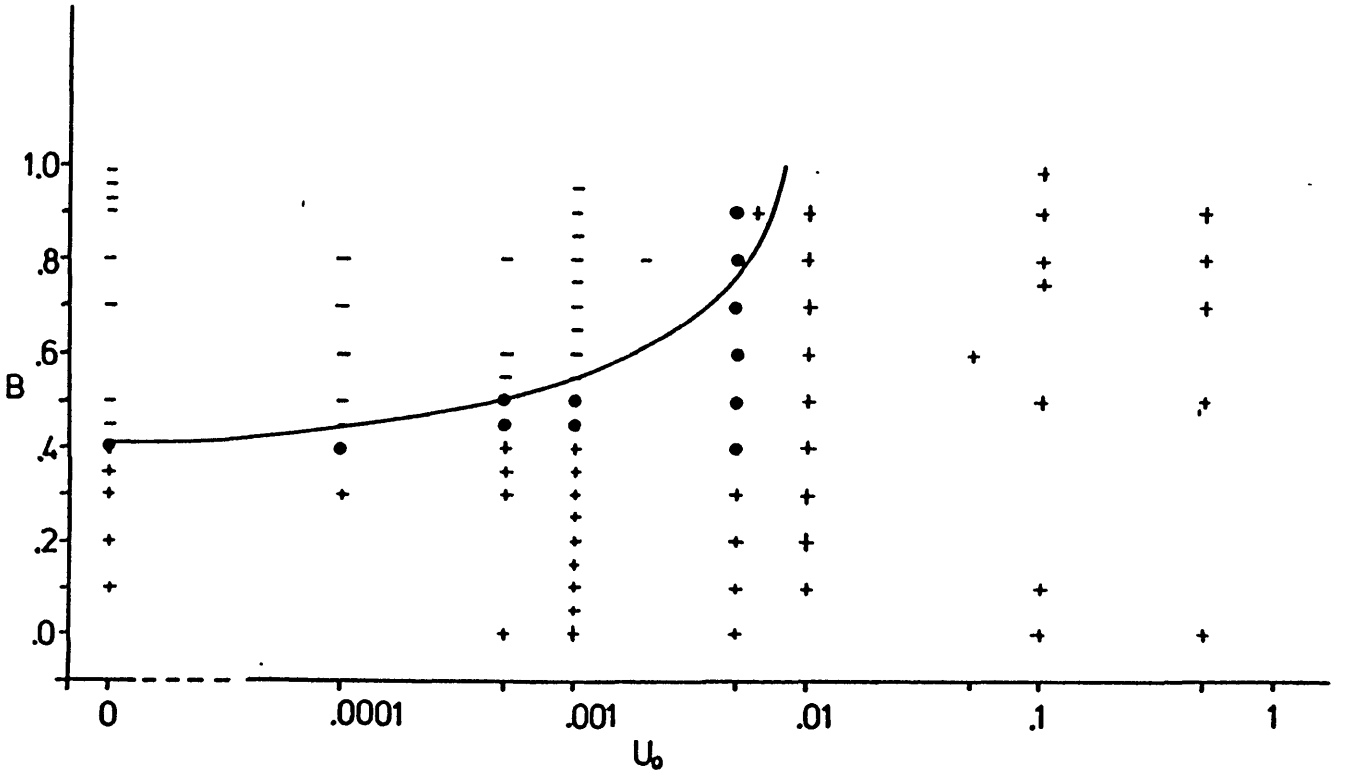


FIG. 3.3 : The final results of the high temperature analysis. The +(-) signs indicate the points examined on the B-U_o plane for which κ is positive (negative). The dots indicate the points for which κ is compatible with zero. The solid curve indicates the approximate position of the κ=0 line.

plane we examined and the corresponding sign of κ. From it we see that the values of B and U_o which any non-trivial field theory can take are restricted. A non-trivial scale covariant $\lambda\phi^4_4$ field theory can only exist for values of B and U_o 'tuned' so that $\kappa=0$, as shown in Figure (3.3).

5. Scale covariance in two dimensions

In this Section we report briefly some preliminary results we obtained in two dimensions. The reason we examined the model for d=2 is in quite a different spirit to that of triviality. As we pointed out in Chapter I, scale covariance could be interesting not only as a non-trivial alternative to canonical theories, but also as a means of examining the problem of non renormalisability. We have seen so far that the proposed change of measure fails to rectify conventional $\lambda\phi^4_4$ to a non-trivial status. We want to investigate whether this failure becomes apparent in aspects of nonrenormalisability as well.

Our line of thinking is the following: We know that conventional $\lambda\phi^4$ in d=2 is a non-trivial superrenormalisable theory which has absolutely no reason to be modified. As was pointed out in Chapter I, in the d=2 case, Sobolev type inequalities indicate that the paths allowed by the quartic interaction are

topologically equivalent to those of the free theory. Thus, perturbations are continuous and the measure need not be modified; i.e. there should be no pseudofree theory distinct from the free case. In terms of our lattice spin analogue model, this means that in the pseudofree case (U_o=0 with B≠0) the theory ought to be non existent for all values of B (i.e. $\kappa < 0$) or belong to the Ising universality class (for d=2, the Ising model is a non-interacting field theory); otherwise a scale covariant pseudofree theory would exist as well as the trivial free one.

We followed the same line of analysis, using high temperature series and Pade approximants to evaluate κ as a function of B when $U_o \equiv 0$. The results are plotted in Fig.(3.4). It is evident that $\kappa < 0$ everywhere; thus scale covariance does not seem to contradict the early (pre-triviality) expectations of its inventor [20,21] at this level of analysis. However, Monte Carlo results are required in order to establish the order of the phase transition and the validity of this conclusion. Moreover, in order to resolve such questions conclusively, one needs to estimate κ with a bigger accuracy than the present one. This can be possibly done with Monte Carlo Renormalisation Group techniques. As the aim of this thesis is to investigate the triviality aspect of scale covariance (and not the renormalisability question) we shall not pursue these questions further.

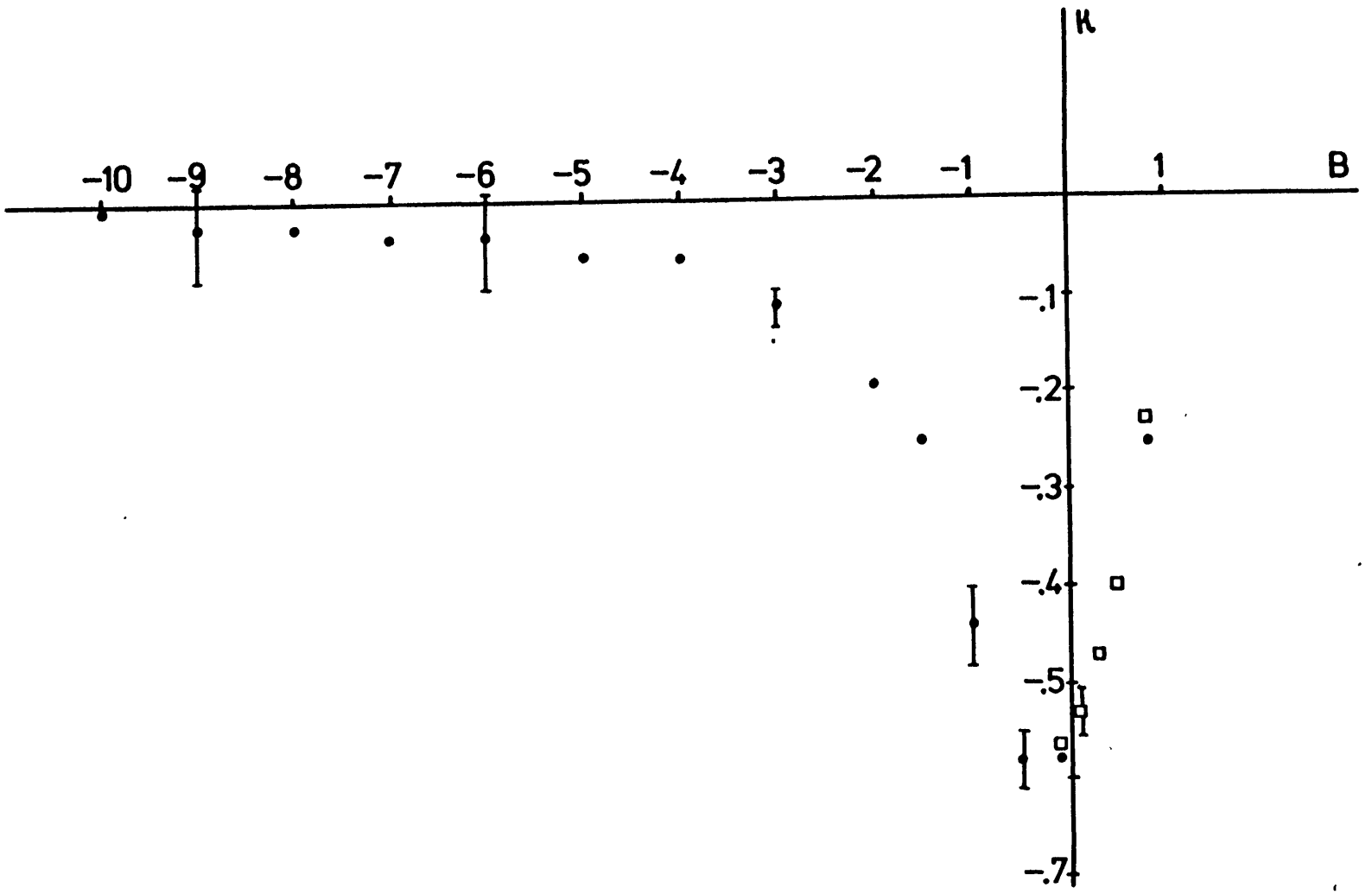


FIG. 3.4 : The variation of κ with B for $U_0 = 0$ and d = 2. The squares indicate results obtained from Method 2; the dots indicate results from Method 3. Results from Method 1 are unreliable due to large statistical errors.

CHAPTER IV

MONTE CARLO ANALYSIS

1. General motivation

As we have repeatedly stressed in the previous Chapter, the results we obtained with the aid of Pade approximants rest entirely on the assumption that our model has a second order phase transition at some inverse temperature K_c for every pair of values (B,U_o). One feels encouraged to believe that this is indeed the case: for any values of (B,U_o) we investigated, the Pade approximants (which are meant to mimic a criticality of second order) seemed to work without problems. The approximants were fairly consistent at least in most, if not in all cases (the only sign of trouble being the violation of universality). However, as we pointed out in Chapter II, the semiclassical Landau approximation indicates that a first order phase transition is possible. Although taking the full quantum effects into consideration will inevitably alter the semiclassical picture, the possibility of a discontinuous transition cannot be ruled out.

This means that the phase diagram of the theory must be worked out. There are various ways that this can be done : (a) solving the model exactly, (b) perturbation

expansions, (c) renormalisation group calculations and (d) Monte Carlo simulations. The first method is unsuitable ; our model is a continuous spin Ising model and so far exact solutions only exist for the one- and two-dimensional discrete spin Ising model. Of the three existing possibilities, Monte Carlo simulations turned out to be the most popular method of obtaining accurate results on phase transitions during the last five years [57]. We shall not describe the Monte Carlo method at all here. A brief discussion of how and why it works will be presented in Chapter VI. In what follows, we shall assume knowledge of the basics of the Monte Carlo technique from the reader.

2. Early Monte Carlo results

The first attempt to clarify the situation was made by Ogielski [37]. Our position towards this work is somewhat critical and our "philosophy" on how to implement Monte Carlo simulations in order to derive information on the triviality of the theory considerably different from Ogielski's. Thus, we shall first summarise his work ; the details can be found in [37]. Monte Carlo simulations were used to investigate thoroughly the order of the phase transition at the following four points of the $B-U_o$ plane : (a) $B=0$, $U_o=1.0$, (b) $B=0.6$, $U_o=1.0$, (c) $B=0.6$, $U_o=0.1$ and (d) $B=0.6$, $U_o=0.01$. Two variants of the Metropolis

algorithm [58] were used. In the first one, a numerical method was used to produce updates from the distribution $d(\sigma)$ of eqn. (2.10) which were accepted or rejected (the Metropolis criterion) with the Ising action $S[\sigma]$ as given in eqn. (2.9). The second variant is the standard one where updates are produced from a flat distribution $d\sigma$ and then they are accepted or rejected with the full $U_o\sigma^4$ action (see next Section, eqn. (4.2)). It was found [37] that results from both variants agree reasonably well at temperatures $T > T_c$ but the second one is more reliable at $T < T_c$.

Ogielski used the internal energy (to be defined below) as an order parameter and studied certain of its properties of convergence to equilibrium from different initial configurations in order to estimate the order of the transition. As a first step, the critical region is located with the aid of the fact that in a stochastic Monte Carlo simulation the order parameter relaxation time grows considerably at temperatures near T_c [59]. Thus, the system is slowly cooled from high to low temperatures and subsequently heated again. The energy was recorded after each temperature change $\Delta T = 0.1$ and a 100 lattice sweeps. The location of the observed hysteresis loops in the energy-temperature plane gives a rough estimate for the value of T_c and their size gives an indication of the order of the phase transition (continuous transitions have much smaller hysteresis

loops than discontinuous ones).

Having located the critical region around T_c, Ogielski then recorded the relaxation to equilibrium of the magnetisation and the internal energy. He used mixed starts, i.e. a 6^3X16 lattice was split into two 6^3X8 subsystems and each was initialy populated by a random and a frozen spin configuration. He then recorded the relaxation to equilibrium of the magnetisation and internal energy in the two halves, for different values of temperature in the critical region. Whenever the order parameters in the two lattice halves converged after about 300 iterations, the transition was termed second order. Such a case must be contrasted to what was intepreted as a first order transition : This was characterised by a distinct coexistence of two phases for up tp 10000 iterations at T_c and slow relaxations (about 4000 iterations) near T_c.

Ogielski supplemented his analysis with an examination of the behaviour of most physical quantities of interest (namely $\chi_{(2)}$, ξ, g_R and the specific heat) in the critical region, using 4^4 lattices and runs with 200,000 to 400,000 configurations. Having found the B=0.6 , U_o=0.01 point displaying non-Ising behaviour, indications of Lebowitz violation and a discontinuous transition and the other three points displaying the opposite behaviour, he concluded that at the points where the field theory exists, it is a trivial one.

Our criticism towards this approach is that although

his simulation is of high enough accuracy to give precise information about the internal energy (the order parameter) and the specific heat , it is insufficient as far as the reported measurements of ξ, $\chi_{(2)}$ and g_R are concerned. For example, despite the huge number of iterations performed, the range of the correlation length turns out to be either larger than the lattice size or smaller than one lattice spacing in the K's of interest ([60] ; see fig. 6(d) and 7(d) of [37]). These estimates turned out to be unreliable although they were obtained with extensive and costly use of the computer. Also, the hysteresis and relaxation method for estimating critical temperatures is very expensive in computer resources and far less accurate than the results which were obtained in Chapter III with the use of the "much cheaper" Pade approximants. Moreover, a non-trivial theory would emerge only for very specific values of the parameters. Such a tuning is impossible to be seen unless a lot of points in the parameter space have been investigated. Thus it is clear that for the four pairs of $B-U_o$ values considered in [37], the order of the phase transition (and only this) has been correctly diagnosed but in order to draw definite conclusions on the theory's triviality, the $B-U_o$ plane must be scanned systematically and more pairs of $B-U_o$ values need to be considered.

3. Monte Carlo calculation of the phase diagram

In this spirit, we followed an approach orthogonal to that of Ogielski. Rather than attempting a high precision Monte Carlo simulation on a few B-U_o points, we opted for a low accuracy simulation for as many values of B and U_o as possible (a high precision simulation on a lot of points of the B-U_o plane would require exceptionally large computing resources). Having already obtained Pade approximants for K_c and κ, we are interested in utilising Monte Carlo simulations in order to determine the order of the phase transistion only. No measurement of g_R or other relevant physical quantities will be attempted. The only aim is to find the phase diagram of the theory and in particular the region for which the transition is second order. This can be achieved with a low accuracy simulation by measuring suitable order parameters. These were chosen to be the absolute magnetization per site and the internal energy per link, defined as

$$M = \frac{1}{N^d} \left| < \sum_k \sigma_k > \right| \qquad (4.1.a)$$

and

$$E = \frac{1}{dN^d} < K \sum_k \sum_{\mu=1}^{d} \sigma_k \sigma_{k+\mu} > \qquad (4.1.b)$$

for a finite lattice of N^4 sites. A slight change of viewpoint is in order here. Instead of simulating our

model with an action and a single site spin distribution as defined in (2.9) and (2.10) respectively (which is the first variant of the Metropolis algorithm used by Ogielski), we found it more convenient to generate a flat spin distribution $d\sigma$ and perform a Metropolis algorithm with action

$$S[\sigma] = \sum_k \left[-K \sum_{\mu=1}^{d} \sigma_k \sigma_{k+\mu} + A\ \sigma_k^2 + U_o\ \sigma_k^4 + \frac{B}{2} \ln\ \sigma_k^2 \right] \quad (4.2)$$

(This is Ogielski's second variant). The lattice size used was 5^4 with periodic boundary conditions. Cold starts were mostly used ;i.e. the field was initially set to a constant non zero value (if $\sigma_k = 0$, the $\ln \sigma_k^2$ term of (4.2) diverges). It turned out that it was adequate to do a 100 lattice sweeps to thermalise the system and another 200 to measure M and E. We have neglected correlations between measurements; thus we have computed the error in the standard way [59] as the ratio of the standard deviation over the square root of the number of measurements. The error was always found to be small.

At first sight it seems unlikely that such a coarse analysis may yield meaningful answers. It is natural to assume that the smallness of the lattice size, the neglect of correlations (which are present in any Monte Carlo calculation) and the low number of iterations would result in big errors in our calculation and thus, render the Monte Carlo analysis unreliable. It has recently

been shown for canonical $\lambda\phi^4$ that this is indeed the case for complicated operators like $\langle\phi\phi\phi\phi\rangle$ (i.e. the evaluation of the four point function ;[10] and [50]), whereas in the case of simple operators like $\langle\phi\rangle$ (used here in the evaluation of the order parameter M) a few iterations on a small lattice turn out to be sufficient [38,60]. This is still true in the case of our scale covariant generalisation. To support this claim, we provide a comparison of Ogielski's results [37] to our own (Table 4.1). It is quite clear that the critical point K_c can be located with an accuracy which is satisfactory for our present purposes. Moreover, a somewhat crude but fairly consistent value for the phase transition "jump" can be obtained.

Of course, the measurement of a finite jump, however big (typical values for the jump range from about 2.5 to 10.0 for M and from 6 to 100 for E !) does not in itself prove the order of the transition. In fact, the rigorous result concerning phase transitions is that for a finite lattice system (i.e. a system described by a finite number of well behaved integrals) no phase transition can occur; a fact which would be reflected in a theoretically infinite Monte Carlo run. It is reasonable though to expect that for a finite system at around K_c, traces of a phase transition can be observed along with certain signals of its order.

We now present our criteria and how we interpreted them as signals of a transition of a particular order:

	LATTICE SIZE	NUMBER OF ITERAT.	K_c	ERROR IN K_c	JUMP IN MAGNETIS.	JUMP IN ENERGY
A	$6^3 \times 16$	10000	0.096	$\pm$ 0.002	~2.50	~ 7.50
B	4^4	200000	0.0966	$\pm$ 0.0005	n/a	~ 8.75
C	5^4	300	0.0975	$\pm$ 0.0015	~2.96	~ 6.00

TABLE 4.1 : Comparison of Monte Carlo results.
A: Ogielski's results with one half of the the lattice initially disordered and the other half ordered. B : Ogielski's results with hot and cold starts done separately. C : Results from the present work.

We know from [38] and [50] that for the canonical theory ($B\equiv 0$) the transition is of second order. If however B is increased sufficiently towards 1, with U_o fixed to an appropriate value, the transition becomes first order[37]. Therefore, for a fixed value of U_o, U_o=const., we started from a high enough value of B (typically B=0.8) and measured the order parameters. Then we moved down the U_o=const. line of the B-U_o plane towards the B=0 line in steps of magnitude $\Delta B=0.2$. We found that for $U_o$small enough, there is a step ΔB for which the behaviour of the order parameters around K_c changes qualitatively. As an example, we describe a representative procedure of obtaining the measurements of relevance: We start at $U_o=0.01$ and B=0.8. From our high temperature analysis, we have an estimate for the critical value of K, $K_c=0.0956\pm 0.0006$. We begin measuring M and E for values well above and below the critical point ($K_c\pm 0.07$) and,as expected, we see that M=0 and E=0 when $K<K_c$ and M~6, E~10 when $K>K_c$. We then repeat the measurements approaching K_c in steps of $\Delta K=0.01$ and observe that the transition jump decreases slowly. As we get nearer the critical region, we decrease the stepsize ΔK in an effort to obtain values of M and E that would interpolate between the zero and non-zero values of the two phases. We found this impossible to do down to step widths $\Delta K=0.0025$; both the M and E curves displayed a discontinuity. We then repeat this process as we move on the $U_o=0.01$ line towards B=0.0

The same behaviour is displayed at B=0.6 and B=0.4. When however B=0.2 or smaller, the order parameters are behaving in a qualitatively different way: as K_c is approached, the M and E curves depart very smoothly from their zero values and it was always possible (to the same or bigger accuracy in ΔK as before) to get values of M and E which interpolated smoothly between their high and low temperature behaviour. The whole proceedure is depicted in Figure (4.1.a) and (4.1.b). Repeating the analysis for even smaller values of U_o we saw even more dramatic differences in the size of the jumps as we vary B; for instance Figure (4.2.a) and (4.2.b). This qualitative difference was interpreted as a signal for the change of the order of the transition somewhere between B=0.4 and B=0.2.

In this manner, we have scanned the B-U_o plane, especially around these points where the high temperature analysis indicates that κ=0. Typical examples of parametric curves of M and E as functions of K (with B as the parameter for a given value of U_o) indicate a range of B values for which the transitions change from discontinuous to continuous and the corresponding K_c ; see also Figure (4.3.a) and (4.3.b). Our results are also in agreement with Ogielski's for the four points he considered.

In Figure (4.4) we indicate the pairs of B-U_o values examined and the order of the transition observed. It is clear that there is an area of tricritical points

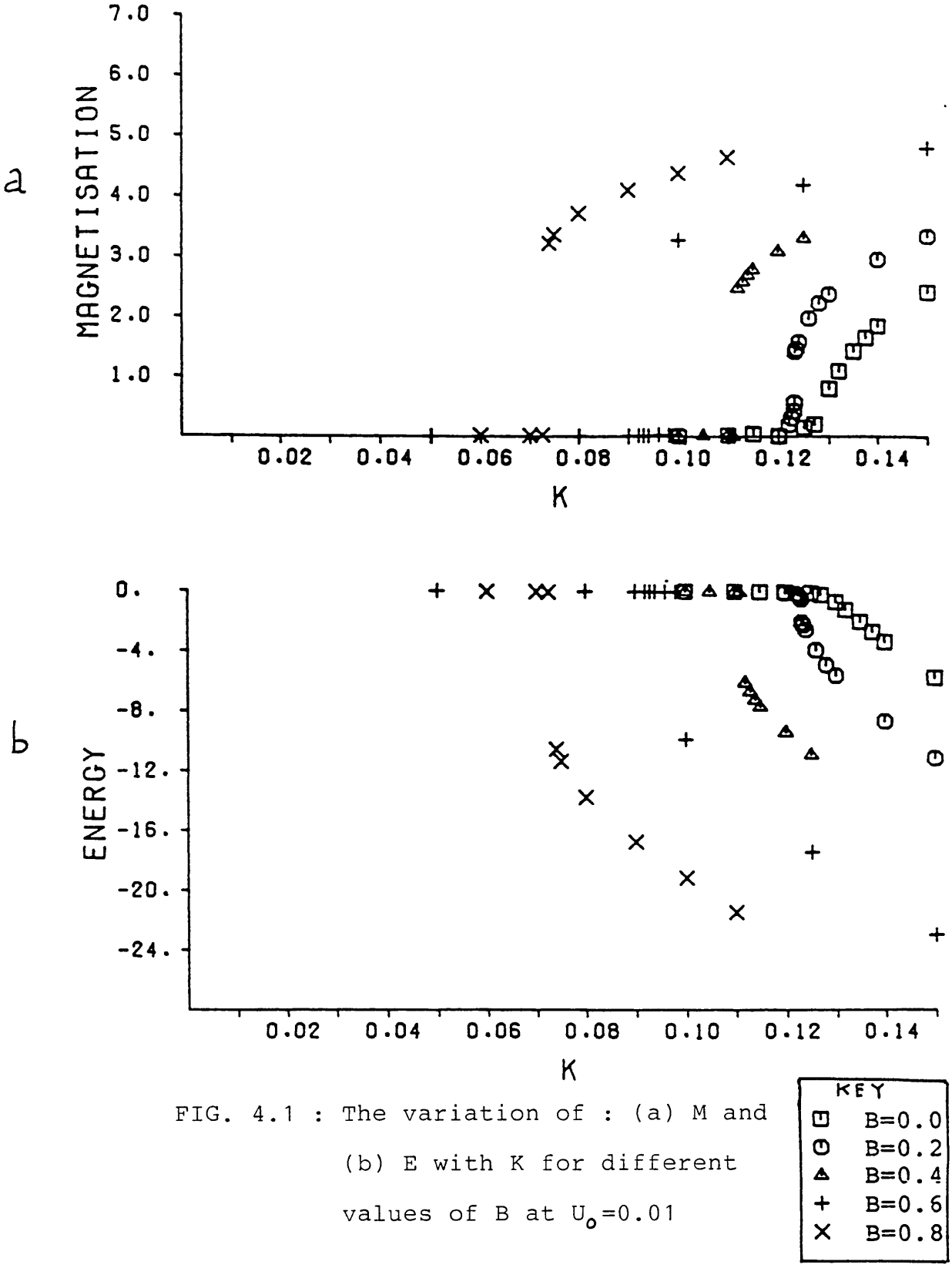


FIG. 4.1 : The variation of : (a) M and (b) E with K for different values of B at U_o=0.01

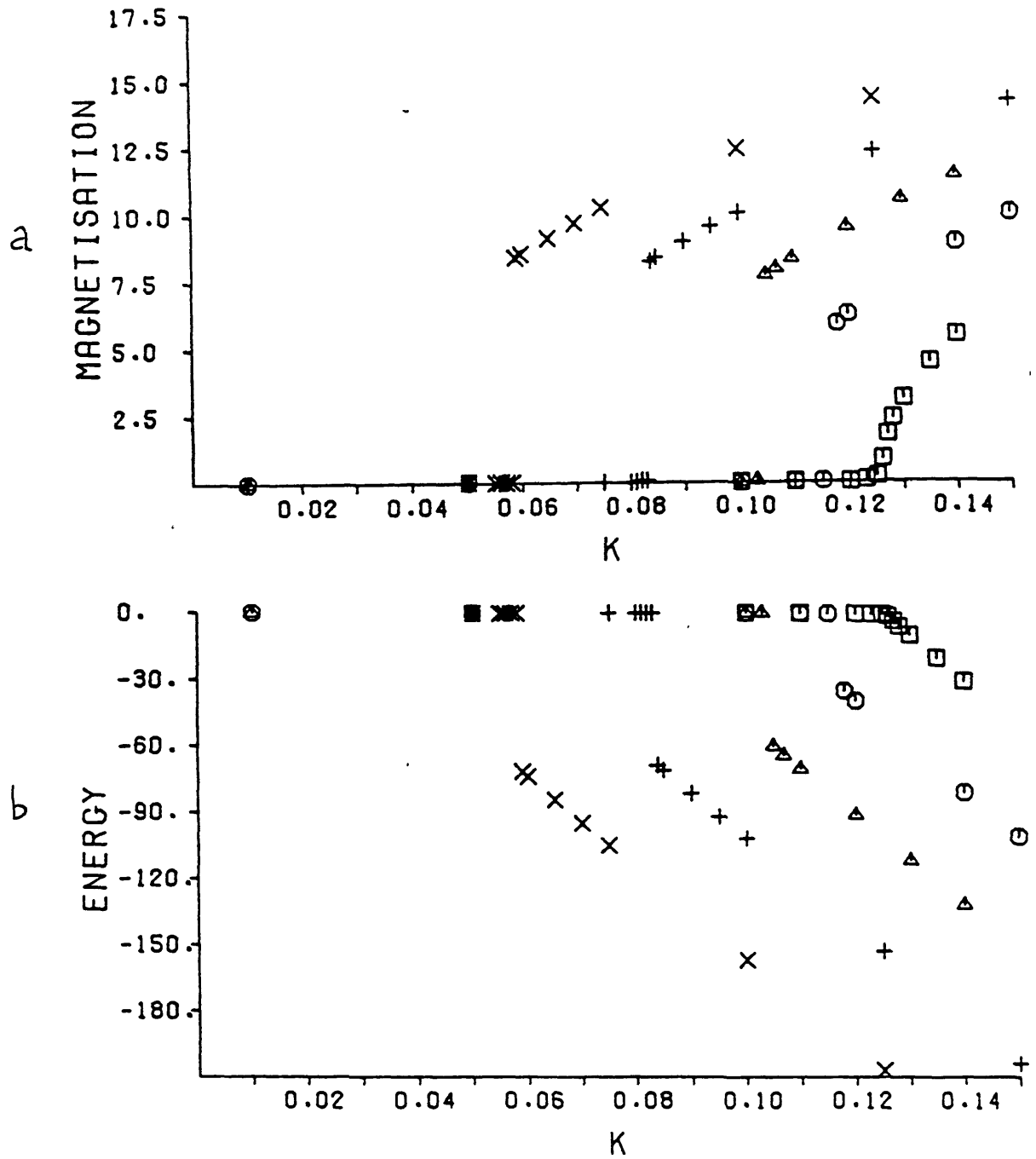


FIG. 4.2 : Same as Fig. (4.1.a) and (4.1.b) for U_o=0.001.

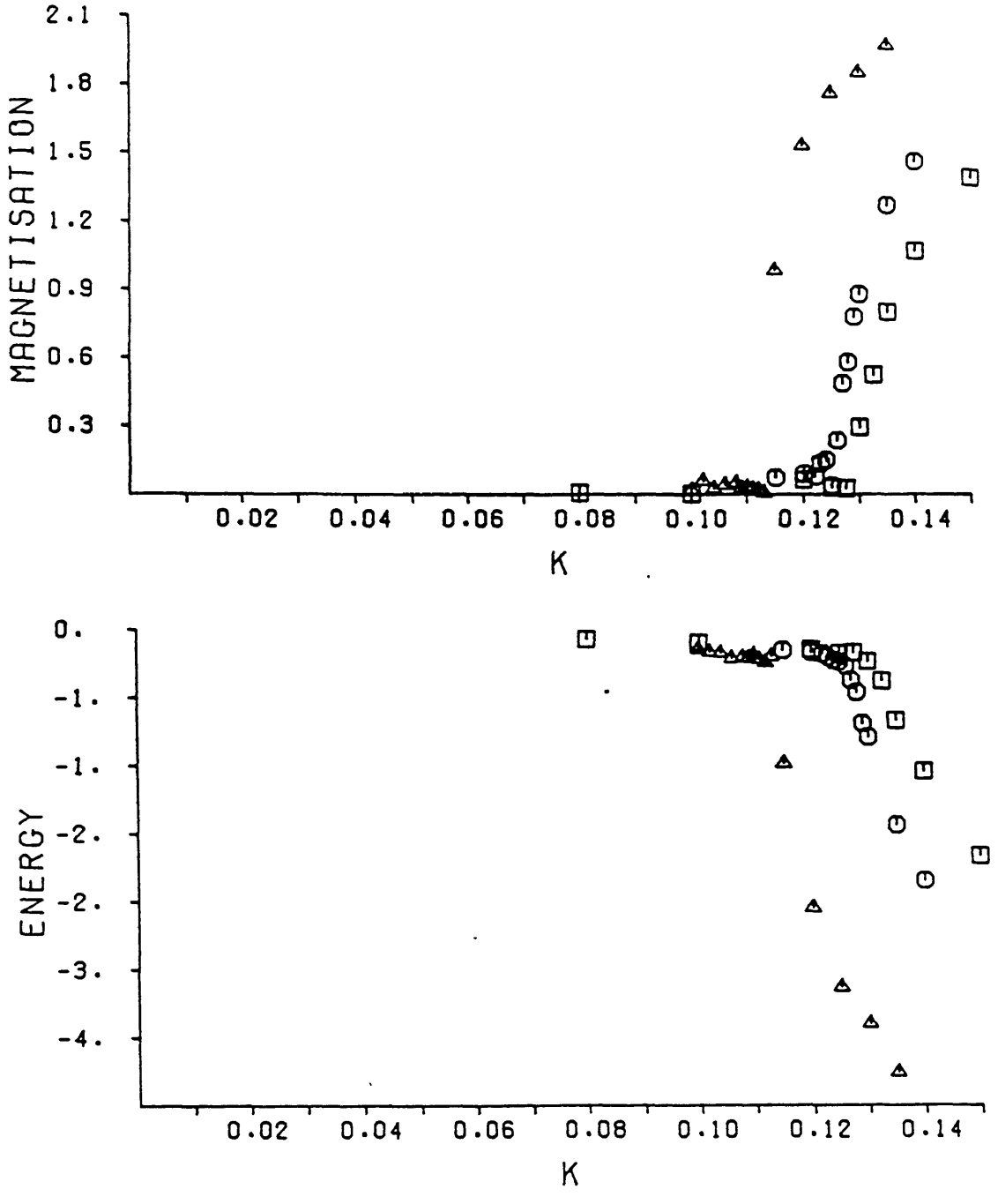


FIG. 4.3 : Same as Fig. (4.1.a) and (4.1.b) for U_o=0.1 .

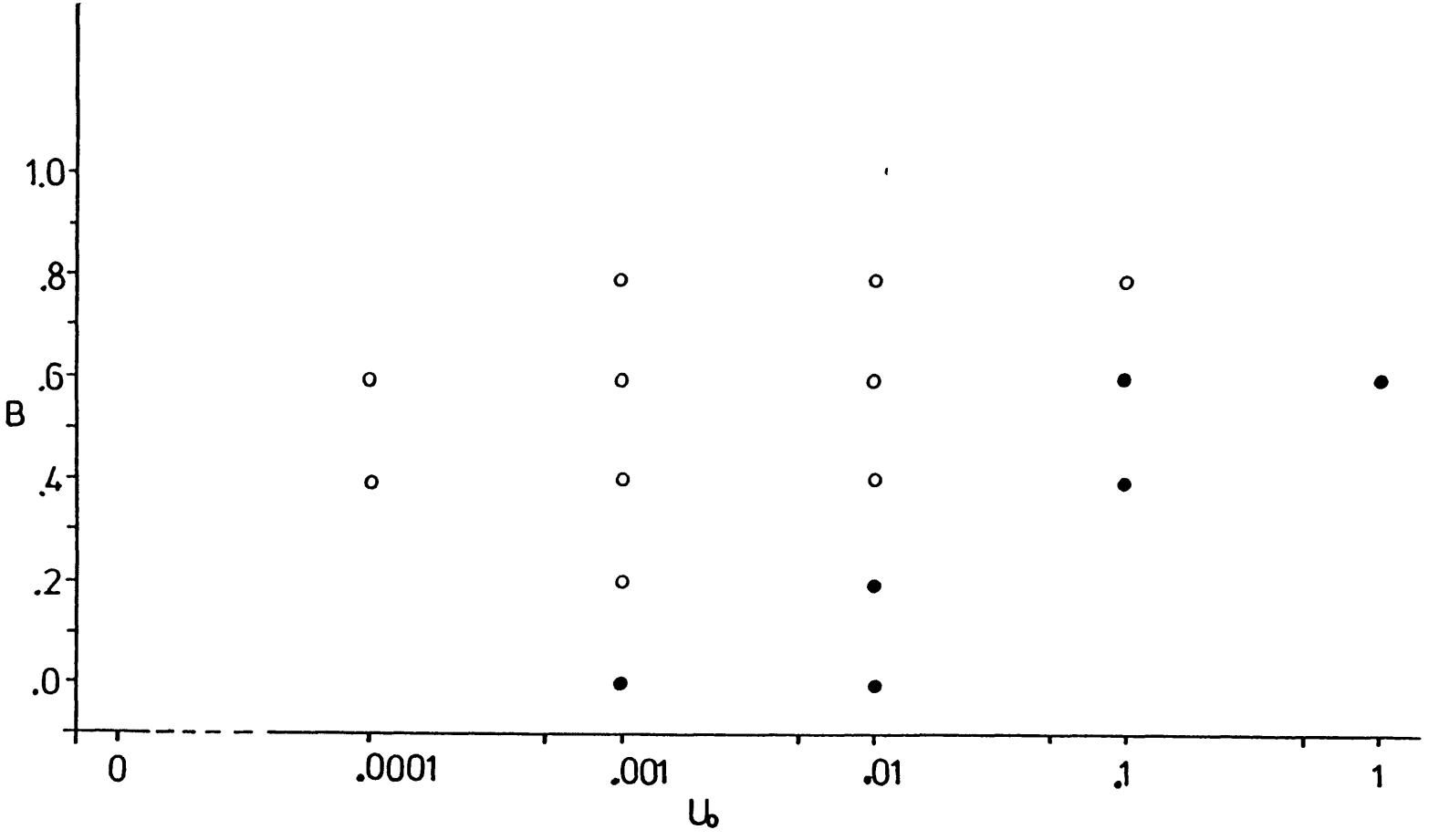


FIG. 4.4 : The open circles indicate the points in the B-U_o plane for which the phase transition is first order ; filled circles indicate second order transition points.

(probably a line) separating the two cases. No continuum field theory can exist in the region of first order phase transitions.

It must be noted here that this analysis would not give convincing results, had we attempted to use it for locating accurately the value of B for which (for a given U_o) the transition would change order. We have only attempted to locate a region (with an uncertainty $\Delta B=0.2$) in which this happens. If we had tried to use this method to perform measurements near the tricritical values of B, we would have been unable to specify whether a jump occurs at K or not. In such cases, it would be necessary to measure the specific heat and perform a finite scaling analysis. As is shown right below, the fact that the region of interest ($\kappa=0$ line) is not near the tricritical region, allows us to draw our conclusions even at this level of low accuracy Monte Carlo analysis.

4. The triviality of scale covariant $\lambda\phi^4$

One can now combine the results from the high temperature analysis of Figure (3.3) with those of the Monte Carlo simulation of Figure (4.4) into one final diagram (Figure (4.5)). From it we deduce that the $B-U_o$ plane is split into two regions, one characterised by a first order phase transition and the other by second order ones. Our earlier Pade approximants measurements of κ were made in both regions under the assumption that

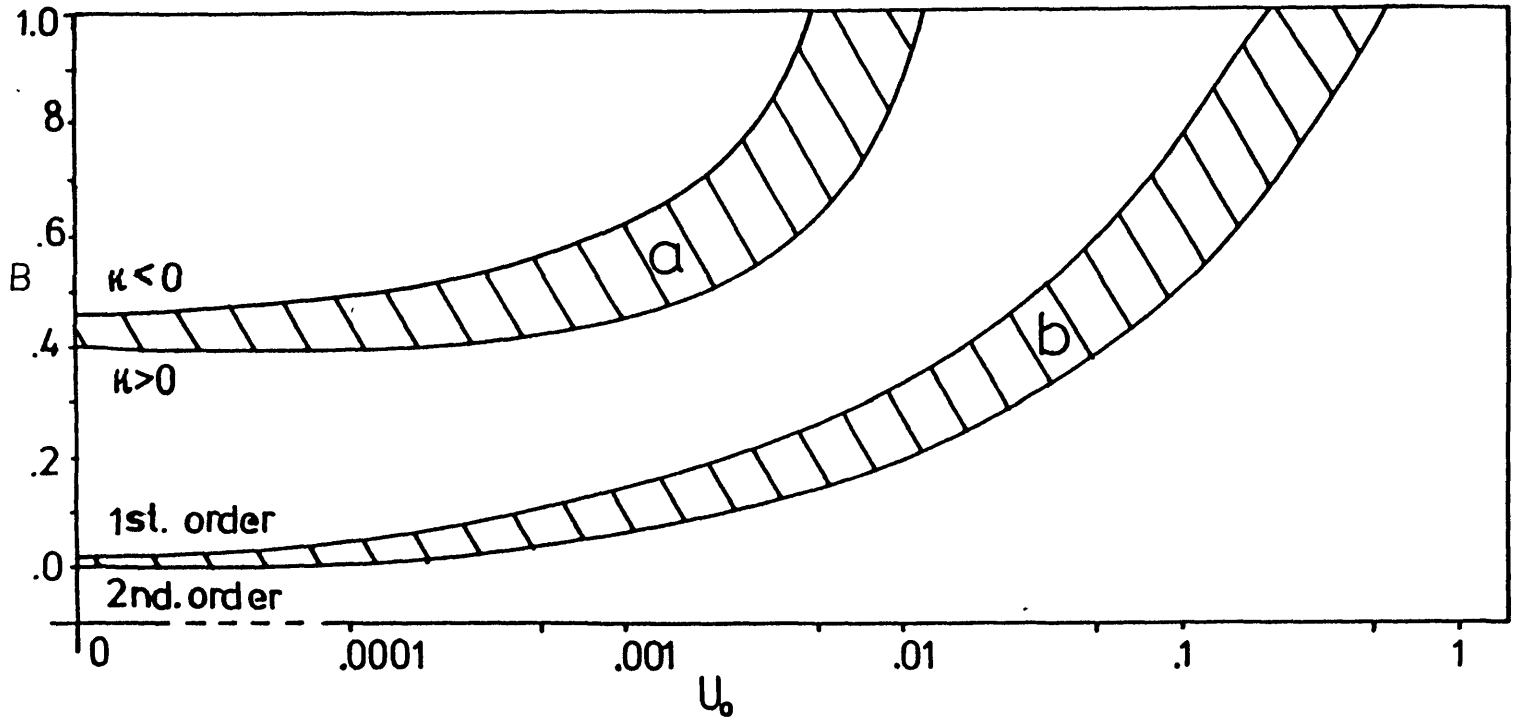


FIG. 4.5 : Division of the B-U_o plane into regions of positive and negative κ and first and second order phase transitions. The shaded areas indicate roughly where (a) the change in the sign of κ and (b) the order of the transition occured.

the transition is always continuous ; therefore our high temperature analysis in the first order region is inapropriate and the results on the values of all the critical exponents (including κ) do not make sense. In the same region the Pade approximants' prediction of K_c was in good agreement with that obtained with Monte Carlo simulations. We do not have any explanation of this. In the region characterised by second order phase transitions, however, the Pade approximants analysis is justified. Naturally, their K_c prediction agrees well with the Monte Carlo one. We see that the value of κ in this region is always positive. In fact, the area of $\kappa=0$ lies so deep inside the no-field theory region, that even a largely improved numerical analysis (e.g. bigger lattices, better error analysis, and longer runs in the Monte Carlo simulation or longer series in the high temperature analysis) is unlikely to affect the qualitative features of this result. Thus, we conclude that scale covariant $\lambda\phi^4$ is a trivial theory.

5. Partial restoration of universality

There is another aspect of the problem which our Monte Carlo simulations have helped clarify and this is the aparent violation of universality. As we have speculated in the previous Chapter, it turns out that the critical exponents vary a lot with B and U_o in or near the region of the B-U_o plane where the transition is

first order or tricritical. It appears that once deep inside the second order phase transition region, the critical exponents vary little with B and U_o and these variations can be attributed to systematic errors, numerical inaccuracies etc. We must point out that throughout the project it was apparent that the χ series behaves a lot better than the $\chi_{(2)}$, μ_2, ξ and g_R series and, consequently, γ is easier to evaluate than ν, Δ and κ. Since we know that their slightly more erratic behaviour is due to the more erratic behaviour of the coefficients of the corresponding series, we have concentrated our attention to the behaviour of the consistently behaving γ exponent.

As an example, we present the results for γ at U_o= 0.01 and for different B values (Figure (4.6)). This is a typical case in which a curve connecting the various γ points seems to be flattening as it moves away from the tricritical region and into the continuous transition area. All other results display a similar behaviour which, without being unambigously universal, does not openly violate univrsality. Besides the case of Fig. (4.6), the worst cases of an apparent universality violation are shown in Figure (4.7.a) and (4.7.b) for the variation of γ and κ with B at U_o = 0.1. Clearly, even in these worst cases, universality violation may be an illusion due to the nearby tricritical points. The idea that tricritical points may influence the behaviour of the high temperature series and their critical exponents

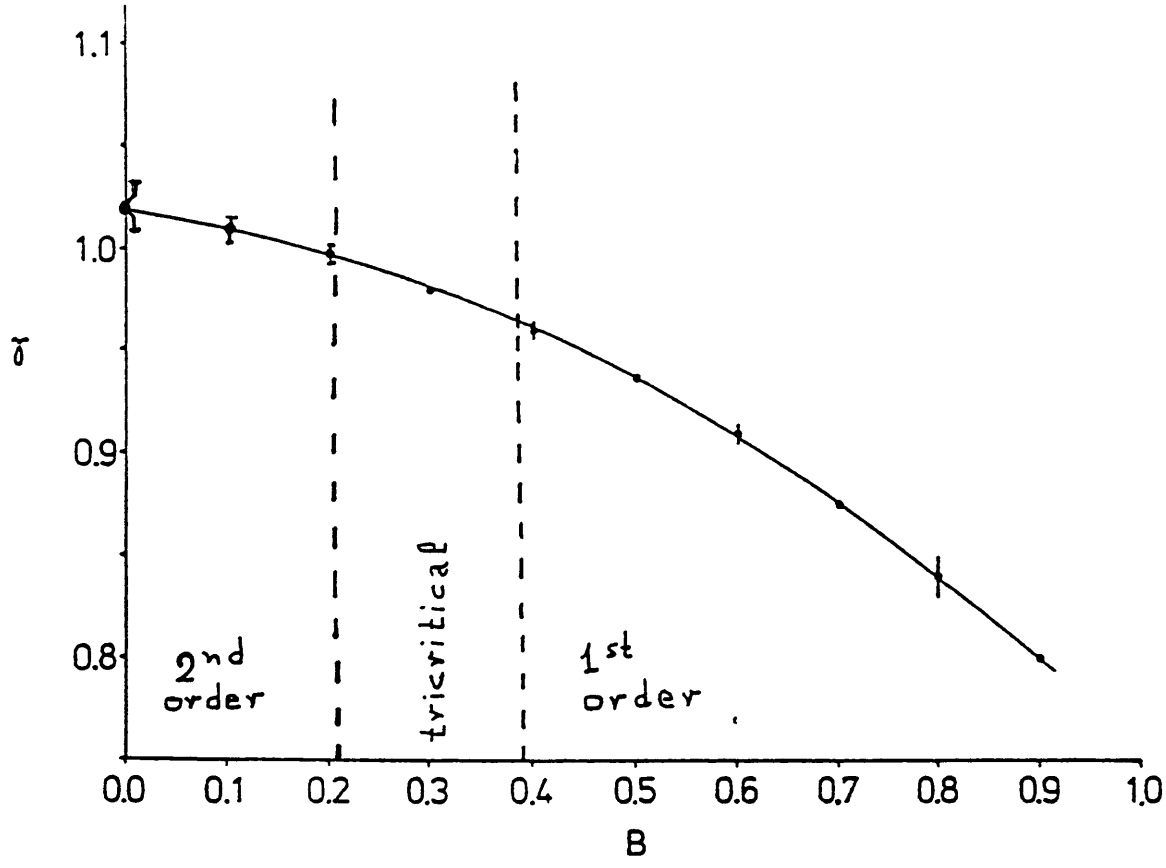


FIG. 4.6 : Variation of γ with B at $U_o = 0.01$. The results are almost universal in the region that they are appropriate ($B \leq 0.2$) .

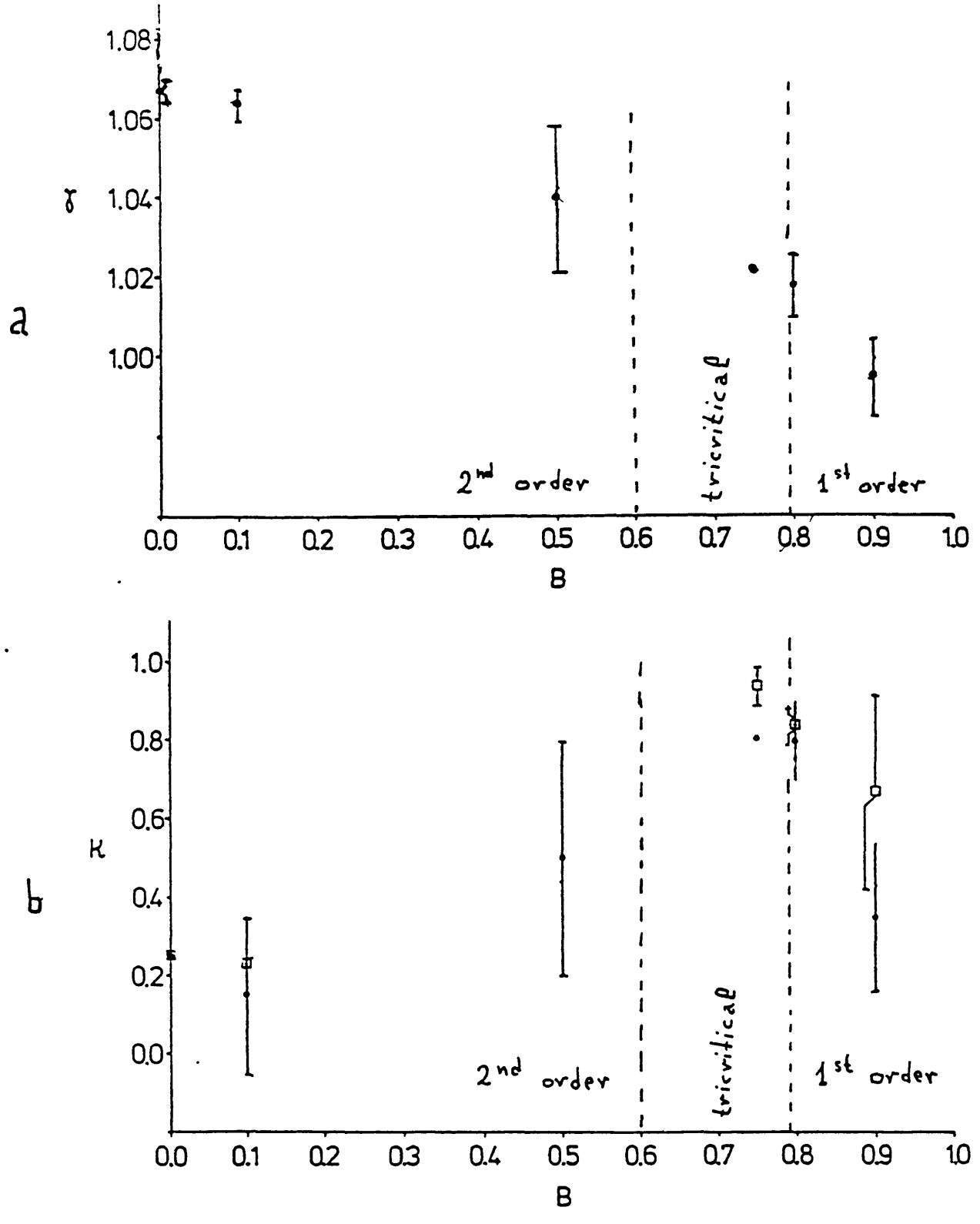


FIG. 4.7 : Same as Fig. (4.6) for (a) : the variation of γ and (b) : the variation of κ , when $U_0=0.1$.

with the result that universality might falsely appear to be violated has resently been proposed by Barma et.al. [61]. This conjecture may be one possible source of "noise". The other is the presence of subdominant singularities, which will be examined in the next Chapter. In any case, we have concluded that the Monte Carlo analysis on the phase structure of the theory has not only rendered it trivial (a result which is contrary to all earlier results on scale covariance) but has also explained the most severe manifestations of universality violation. Although universality has not been proved, the Monte Carlo refinement on the data showed that our results are not incompatible with it.

CHAPTER V

CONFLUENT SINGULARITY ANALYSIS

1. On the presence of confluent singularities

So far, we have occasionally been stressing the fact that the characteristic critical behaviour

$$F(K) \sim (K_c - K)^{\varepsilon} \tag{5.1}$$

of the correlation functions is only a conjecture. It is a justified one, as it is suggested by Renormalisation Group analysis [40,45]. It is however, nothing else but the dominant divergent behaviour ; subdominant power-law divergencies of the form

$$F(K) = C_0(K)(K_c-K)^{-\varepsilon_o} + C_1(K)(K_c-K)^{-\varepsilon_1} + \ldots \tag{5.2}$$

are expected [62]. Here, $C_i(K)$ are the non-universal amplitudes of the theory, which are regular in K. They also depend on the bare parameters (like B, U_o) but they are not necessarily analytic for all their values. We also define ε_o to be the dominant exponent and the rest of the ε_i's to be confluent singularities ;(i.e. $\varepsilon_o > \varepsilon_1 > \ldots$). Another posibility is the presence of logarithmic

factors of the form

$$F(K) = (K_c-K)^{\varepsilon}[\ln(K_c-K)]^{\lambda} \qquad (5.3)$$

Behaviours of the form (5.2) and (5.3) can even occur cumulatively. We shall see in a latter Section of this Chapter how they introduce systematic errors in the Pade evaluation of the dominant singularity. In any case, as B and U_o vary, the analytic parts $C_i(K)$ will vary with them. This results in the variation of the relative strengths of the confluent corrections to scaling. It is conceivable that in the light of the previous analysis, the slightest departures from universality of the values of ε_o is an artefact of the neglect of confluent singularities. Moreover, since taking confluent singularities into account may alter the Pade estimates for ε_o, it may turn out that the physical picture we have in Figure (4.5) is inaccurate. It is unlikely but in principle possible that the two "bands" of Fig. (4.5) (i.e. the tricritical points and the κ=0 points) may overlap. This will alter the conclusion on the triviality of scale covariant $\lambda\phi^4$. In this Chapter, we shall investigate the effects of a power law confluent correction (eqn. (5.2)) on our results. We shall again neglect logarithmic corrections such as those of eqn(5.3). This is because series extrapolation techniques turn out to be somewhat inefficient in

detecting logarithmic corrections in relatively short series ([54,63]).

There are quite a few methods for detecting confluent singularities. As an example, we metion the differential approximants (see [64] and references therein) and the inhomogeneous partial differential approximants [65]. As these methods turn out to be relatively inefficient unless the series are long [63], we will use a third method which is known to work even when the series are short [66,67]. This method will be analysed fully in Section 3.

2. The dispute on universality limitations

Before presenting the method we used and the results we derived, we wish to refine the notion of universality. The universality hypothesis is that all critical problems may be divided into classes differentiated by (a) the dimensinality of the system; (b) the dimension of the local variables in the action; (c) the symmetry group of the coupling between the local variables (which is the symmetry of the order parameters) and (d) perhaps other criteria [39,68]. The last criterion (d) is, of course, very general and leaves a lot of room for different interpretations of the validity and generality of the universality hypothesis. This is especially so in the case of $\lambda\phi^4$ theory, whether canonical or scale covariant. We have shown that this theory is a model with an Ising-

like nearest neighbour interaction. Unlike the original Ising model, however, $\lambda\phi^4$ has a spin on each lattice site the value of which varies continuously from $-\infty$ to $+\infty$. Its actual value is determined stochastically by the single site spin distribution $d\mu(\sigma)$ of eqn. (2.10).

Let us first examine the canonical case ($B\equiv 0$). When $U_0=0$, the spin distribution is clearly that of a Gaussian model. When $U_o \to \infty$, it turns out that $d\mu(\sigma)$ becomes symmetrically double peaked (δ-function peaks) and so it represents te spin-$\frac{1}{2}$ Ising model [69]. In the case of the pseudofree ($U_0\equiv 0$) scale covariant theory, we again have the Gaussian model when $B=0$ and a spin-$\frac{1}{2}$ Ising model when $B \to \infty$ [29]. The question that arises is whether in these cases the continuous spin Ising model remains in the same universality class as it interpolates smoothly between the Gaussian and the spin-$\frac{1}{2}$ Ising model. We shall see shortly how such an interpolation offers a natural way through which the fourth and most intangible notion that differentiates universality classes may arise (recall that this notion was just "other criteria").

Two contradicting answers have been given to this question. The first one comes from the work of Fisher and his collaborators [56], who analysed two models that extrapolate smoothly between the Gaussian and the spin-$\frac{1}{2}$ Ising model. One was Klauder's pseudofree theory and the other the double Gaussian model. They used partial differential approximants to analyse the series for the three dimensional case and for the multicritical point of

the parameter space. Their results imply Ising-like universality over the whole range of values of the model's parameters. Also, the values of both the primary critical indices and the confluent singularity for the susceptibility χ turn out to be universal over the two models. Thus, they conclude that universality is valid in its strongest sense for the interpolating models.

A different approach is that of Baker and Johnson who examined the universality problem whithin the same model, namely canonical $\lambda\phi^4$ in two dimensions, and investigated whether the critical index of the susceptibility χ is universal for all values of the bare coupling U_0. They adopt the conjecture [46] that the shape of the single site spin distribution $d\mu(\sigma)$ and certain properties of the amplitude of the correlation length are responsible for limitations on the model's universality. In particular they note that near K_c^-, the correlation length behaves like

$$\xi = D_+(U_0)\ [1-K/K_c(U_0)]^{-\nu} \qquad (5.4)$$

and it turns out that there is a "borderline" value of U_0 (which is $U_b=[\Gamma(\frac{3}{4})/\Gamma(\frac{1}{4})]\simeq 0.114$) for which $A(U_b)=0$ and D_+ diverges. (Recall that A is a function of U_0 defined through eqn. (2.7).) Now they distinguish five regions of U_0 values for which $\lambda\phi^4$ can be expected to have different critical behaviour. They are :

(i) $U_0 = 0$, for which $d\mu(\sigma)$ is the distribution of the Gaussian model

(ii) $0 < U_0 < U_b$, for which $d\mu(\sigma)$ is symmetrically single peaked

(iii) $U_0 = U_b$, the "borderline case"

(iv) $U_b < U_0 < \infty$, for which $d\mu(\sigma)$ has a minimum at $\sigma=0$ and two symmetric round peaks

(v) $U_0 = \infty$, for which we have the Ising model

In [46], Baker and Johnson studied the U_b case. They examined the χ series with and without taking the confluent singularities into account, for plane square and triangular lattices. They found that $\gamma=1.955\pm0.065$ which is different from the Ising model's value (at $U_0=\infty$) $\gamma=1.75$ [70]. Therefore, universality is not valid over the whole U_0 range $(0,\infty)$. This result suggests that the behaviour of the single site spin distribution and the amplitude of ξ may provide the "other criteria" for distinguishing different universality classes. It is possible that only within each of the five regions of U_0 values referred to above, the theory obeys universality. Thus, the model's real parameter space may consist of different universality regions.

Using their partial differential approximants, Fisher and collaborators claim that this is not so. In particular, they examined the scale covariant pseudofree and the double Gaussian models in two dimensions [61]. They concluded that certain multicritical properties suggested by their analysis imply universality over the

whole range of the bare parameter for both models. Despite the fact that they also found "borderline" values of the bare parameter for which both models had $\gamma \sim 2$, they regarded this result an anomaly. They propose that the presence of the anomaly may be explained by the fact that in the full Hamiltonian space the manifolds corresponding to all the border models under consideration lie "close" to a tricritical subspace. The anticipated proximity of the tricritical region to the border model is regarded as the source of an overestimation of γ. As this conjecture is only supported by weak qualitative plausibility arguments [61], Baker and Johnson have recently refuted it on similarly qualitative plausibility lines [71].

In the spirit of Baker and Johnson, we examined the behaviour of the scale covariant spin distribution $d\mu(\sigma)$ under variations of B and U_0. Given $d\mu(s)$ from eqn. (2.10), we define $M(\sigma)$ through

$$d\mu(\sigma) = M(\sigma)\, d\sigma \qquad (5.5)$$

Ogielski [37] has given examples of some characteristic shapes of the function $M(\sigma)$ for a few values of B and U_0. We have worked out all the regions of the B-U_o plane for which $M(\sigma)$ has different "characteristic shapes". By this we mean that we have ignored the fine details of the function $D(\sigma)$ (i.e. saddle points, widths etc) and only paid attention to the number of its peaks as well as their sharpness (i.e. rounded or infinite peaks). The

result, depicted in Figure (5.1), is the separation of the B-U_o plane into different candidates of universality classes. The dividing curve turns out to be the locus of points satisfying

$$A(B,U_0)^2 - 4BU_0 = 0 \quad , \text{ with } A < 0 \qquad (5.6)$$

It has been located numerically. As we do not have any knowledge of the singularities of the amplitudes of ξ, the possibility of borderline models has been ignored.

The object of this thesis is not to examine the universality issue. We have only presented the whole situation in order to demonstrate that the question of universality is still open and that a definite answer is not easily obtainable. Thus, our primary concern is to examine the influence of the confluent singularities on the result we have obtained ; i.e. the triviality of scale covariant $\lambda\phi^4$. It is a matter of secondary interest (which, however, may in principle be obtained as a by-product of our analysis without extra labour) to see whether a confluent singularity analysis may have any effect on the weak conclusions we derived in Chapter IV regarding the model's universality.

3. Confluent singularities and Pade approximants

The most suitable method for obtaining a confluent

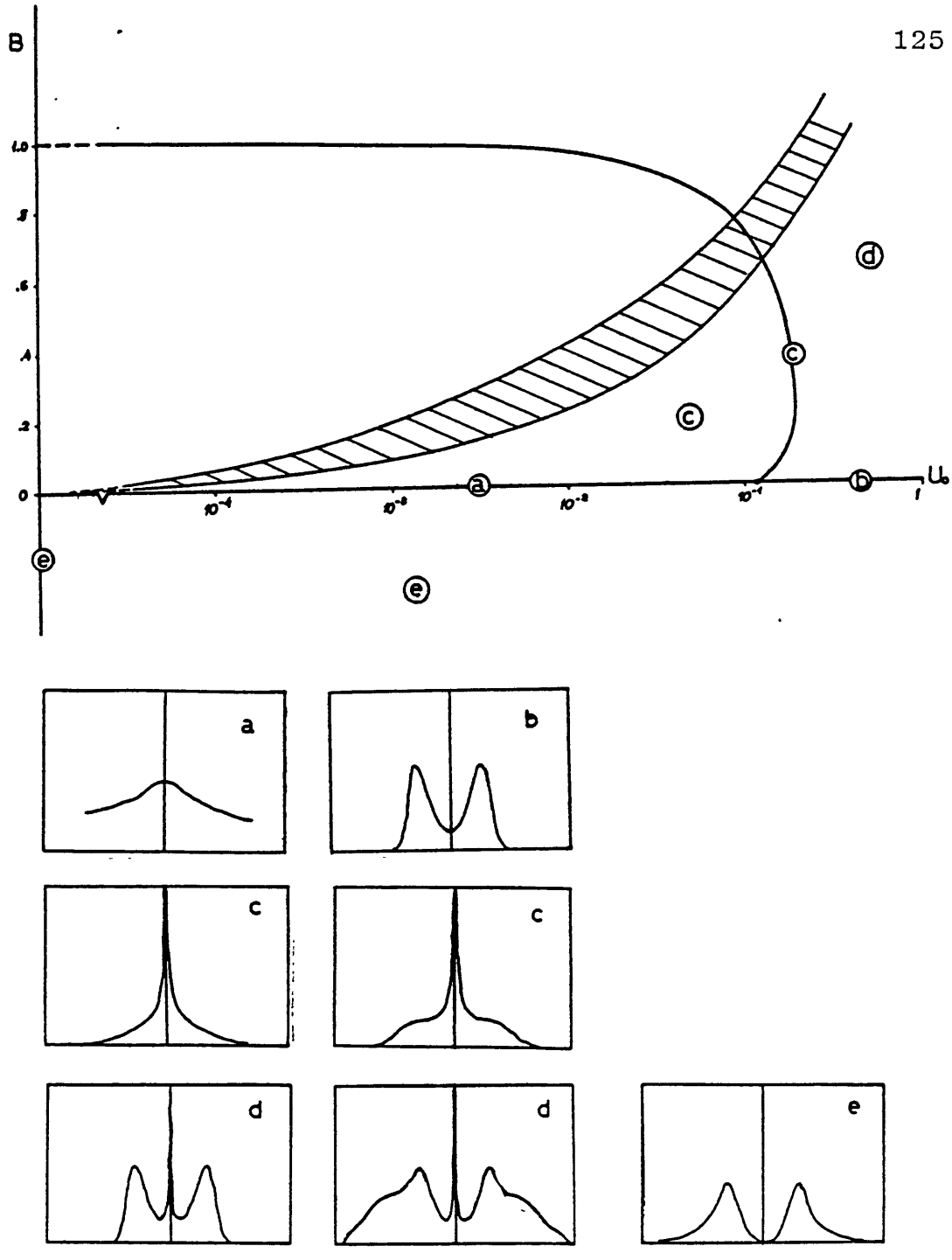


FIG. 5.1 : Separation of the B-U_o plane into different regions according to the five characteristic shapes of the single site spin distribution. The shading marks the tricritical region.

singularity structure from a short high temperature series has recently been proposed by Adler et.al. [66,67]. It is essentialy a generalised variant of the D-log Pade approximants. We start by specifying our conjecture for the critical behaviour of some correlation function F(K) ; it is to behave like eqn. (5.2) truncated after the first two terms. After some trivial algebra and an expansion of the analytic functions $C_i(K)$ in powers of (K_c-K), like

$$C_i(K) = c_i^{(0)} + c_i^{(1)}(K_c-K) + c_i^{(2)}(K_c-K)^2 + \ldots \qquad (5.7)$$

we may reexpress the critical behaviour in the form

$$F(K) = a(K_c-K)^{-\varepsilon_0} [\, 1 + a_0 (K_c-K)^{D_1} +$$

$$b_1(K_c-K) + a_1(K_c-K)^{D_1+1} + b_2(K_c-K)^2 + a_2(K_c-K)^{D_1+2} + \ldots] \qquad (5.8)$$

where

$$D_1 \equiv \varepsilon_0 - \varepsilon_1 \qquad (5.9)$$

and a, a_i's and b_i's are constants in K, which depend on B and U_0 and are expressible in terms of the $c_i^{(m)}$'s of eqn. (5.7). In (5.8) we have only kept the first three terms of the expansion (5.7). The fact that we want ε_1

to be a confluent singularity means that it must satisfy both $\varepsilon_1 > 0$ and $\varepsilon_1 < \varepsilon_0$ which restricts D_1 in the region $\varepsilon_0 > D_1 > 0$.

The method of Adler et.al. will now be described. They assume [66] that the ratio of the amplitude a_0 to the other amplitudes (a_1, a_2, b_1, etc) is sufficiently large to allow us to truncate (5.8) even further :

$$F(K) = a(K_c-K)^{-\varepsilon_0} \left[1 + a_0(K_c-K)^{D_1} \right] \qquad (5.10)$$

From expression (5.10) we see that a biased D-log Pade analysis of F(K) (i.e. Method 3 of Chapter III) in the presence of a confluent singularity, probes a behaviour like

$$(K_c-K)\,(F'/F) = \varepsilon_0 - \frac{a_0 D_1 (K_c-K)^{D_1}}{1 + a_0(K_c-K)^{D_1}} \qquad (5.11)$$

which reduces to eqn. (3.15) and Method 3 when $a_0=0$. Now, however, the term $(K_c-K)^{D_1}$ is not analytic when D_1 is not an integer and Pade approximants are not expected to converge well at branch points such as K_c. Thus, the presence of confluent singularities may have been a source of systematic errors in the previous analysis.

The next step in the method is to change variables from K to y, which is defined by

$$y = 1 - (1 - K/K_c)^D \tag{5.12}$$

where D is a new free parameter. Reexpressing F(K) in terms of y we get

$$F(K(y)) = a\, K_c^{-\varepsilon_0}\, (1-y)^{-\varepsilon_0/D}\, [\, 1 + a_0\, K_c^{D_1} (1-y)^{D_1/D}\,] \tag{5.13}$$

As $K \to K_c$, $y \to 1$ and the D-log Pade analysis in terms of the new variable y now consists of approximating the function

$$G_D(y) = D\,(1-y)\, \frac{d}{dy}[\, \ln F(K(y))\,] \tag{5.14}$$

which, given (5.12) behaves like

$$G_D(y) = -\gamma + \frac{\tilde{a}_0\, D_1\, (1-y)^{D_1/D}}{1 + \tilde{a}_0\, (1-y)^{D_1/D}} \tag{5.15}$$

where $\tilde{a}_0 \equiv a_0 K_c^{D_1}$. Obviously, the choice $D=D_1$ reproduces the usual D-log Pade evaluation of ε_0 (c.f. eqns. (5.12) and (5.15)). The cases of interest are those for which $(1-y)^{D_1/D}$ is analytic. This is so when $D=D_1/k$ with k integer. For D close to D_1/k, we may linearise (5.15) in $D-D_1/k$ and retain the leading terms as $y \to 1$, to get

$$G_D(y) \approx \varepsilon_0 + \tilde{a}_0\, k^2\, (1-y)^k\, \ln(1-y)\, (D-D_1/k) + O((1-y)^k) \tag{5.16}$$

Any Pade approximant of $G_D(y)$ is an estimate of ε_0 and forms, for different values of D, a trajectory on the ε_0-D plane. The above expression (5.16) implies that the trajectories of different order Pade approximants should intersect with small slopes at the points ($D=D_1/k$, $\varepsilon_0=\varepsilon_{0exact}$) of the ε_0-D plane. This ideal picture is smeared by finite series effects and higher confluent terms. In practice [66,67], one observes a convergence of the different approximants in a region of the ε_0-D plane for $D \approx D_1$ which allows a better estimation of ε_0 than the one obtained with the simple biased D-log Pade method. The resulting estimate of D_1 is very unreliable. This is analogous to the situation of the simple D-log Pade approximants which provide us with excellent estimates for K_c but rather poor results for ε_0.

4. Results from the confluent singularity analysis

We will now apply the method of Adler et.al. to our high temperature series for the scale covariant $\lambda\phi^4$ theory, in order to establish whether neglecting confluent singularities is a justifiable approximation or not. There is one problem in applying the method of the previous Section and this the fact that K_c must be a

known input parameter. As we do not know the critical temperature exactly, the method is expected to work less accurately than in the cases it was originally used [66,67]. For models with unknown critical temperature, the standard way out is to use the K_c estimate from the original Pade analysis. This was successfully implemented for $\lambda\phi^4$ in two dimensions [46] and the Ising model in three dimensions [72]. We have used our Pade $K_c$estimates which were always accurate to four or five significant digits. Moreover, we shall describe an improved version of the method which sometimes gives better results as we vary $K_c$slightly.

It would be desirable to repeat the complete analysis of Chapter III using the Adler et.al. method. This is very unrealistic since for every point of the $B-U_o$ plane and for each critical exponent, one has to make multiple measurements for different values of D, in order to plot the Pade trajectories on the ε_0-D plane. If, on top of this, one wants to vary K_c slightly in order to be optimally confident about the answer, the restrictions on computer resources become inhibitive. Such considerations have enforced us to consider very few points of the $B-U_0$ plane. We have also examined the susceptibility series only, which, as we mentioned in the last Chapter is the more reliable one. The assumption is that if the results turn out to be uninfluenced by the presence of confluent singularities for χ, then the whole analysis of Chapter III ought to be reliable. If not, we

must also investigate the other series .

Typical results are presented for the points B=0.1, U_0=0.05 and B=0.3, U_0=0.15 . Our original estimates were

$$K_c=0.13088(0) \ , \ \gamma=1.046(4)$$

for the first, and

$$K_c=0.13405(4) \ , \ \gamma=1.066(4)$$

for the second point. Using these K_c values as input parameters and the method of the last Section, we obtained

$$\gamma=1.0506(18) \ , \ D_1=0.75(15)$$

for the first, and

$$\gamma=1.0689(7) \ , \ D_1=0.9(1)$$

for the second (B,U_0) point. These results have benn obtained from Figure (5.2.a and b.). The errors have been estimated in the standard "windowing" fashion of Adler et.al. Thus they are very subjective.

The next step is to investigate the sensitivity of these results to slight variations of the input K_c. We repeated the analysis for a few new K_c values (typically introdocing a small deviation $\delta \sim 0.001$ from the original estimate) and found a significant instability of γ. To see how this arises, we have repeated the analysis of Section 3 with

$$y = 1 - (1 - K/(K_c \pm \delta)) \qquad (5.17)$$

to find, not surprisngly, that

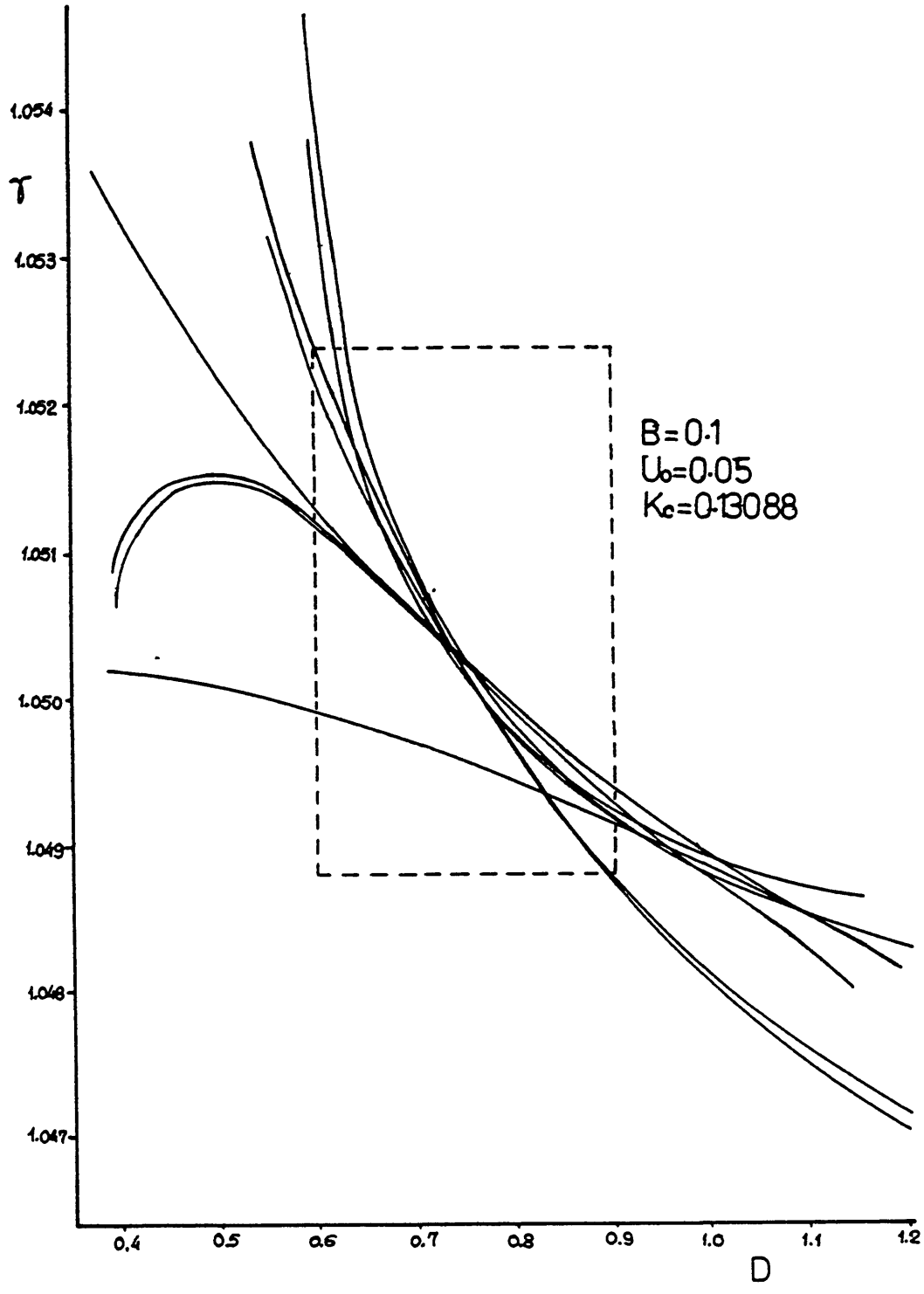


FIG. 5.2.a : Plots of $\gamma(D)$ obtained with the [L/M] Pade approximants ($3 \leq L, M \leq 6$). The window indicates the estimated region of convergence.

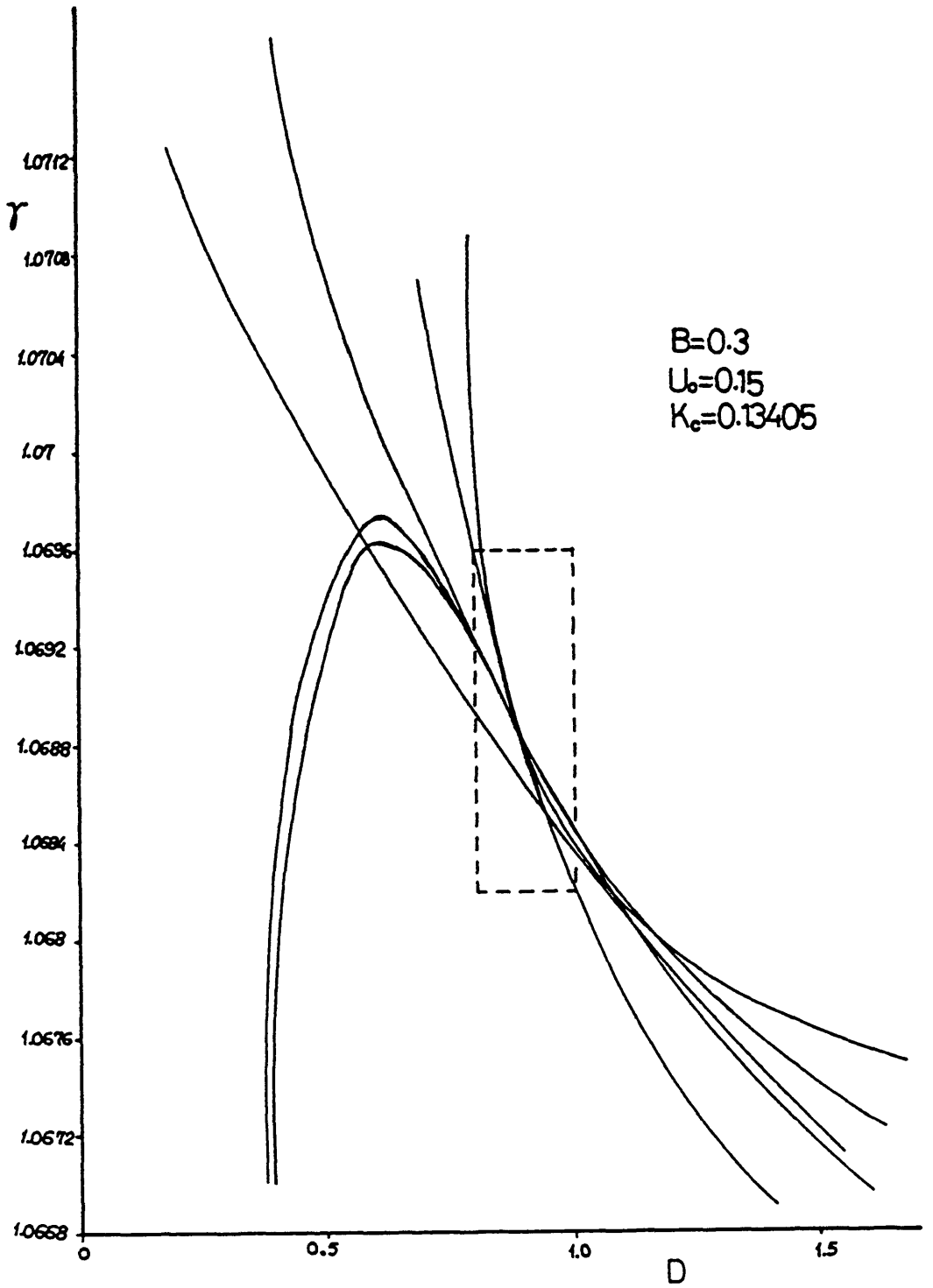


FIG. 5.2.b : Same as Fig. 5.2.a for a different B-U_o point.

$$G_D(y) = \varepsilon_0 - \frac{\tilde{a}_0 D_1 (1-y)^{D_1/D}}{1+\tilde{a}_0(1-y)^{D_1/D}} + C(y)\delta \qquad (5.18)$$

where we have linearised in δ. The coefficient C depends in a complicated way on a_0, D_1, K_c, γ and grows as $y \to 1$. If a_0 is not as large as it has originally been anticipated, then the third term of (5.18) wins over the second one and systematic errors occur. Luckily, this also results in large errors that signal the unreliability of an input $K_c \pm \delta$.

In order to find a way round such uncertainties, we have introduced the following variant to the method: If small δ values result in big instabilities of γ, this is due to the smallness of a_0. It may then be that the original assumption of Adler et.al. that a_0 is the largest amplitude in eqn. (5.7) is not always true. In such a case, the next non-analytic term with amplitude a_1 may be important. Repeating the analysis with the a_1 rather than the a_0 term surviving in (5.10) gives

$$G_D(y) = \varepsilon_0 - \frac{\tilde{a}_1(D_1+1) (1-y)^{(D_1+1)/D}}{1 + \tilde{a}_1(1-y)^{(D_1+1)/D}} \qquad (5.19)$$

with $\tilde{a}_1 \equiv a_1 K_c^{D_1+1}$. This implies that there may be another convergence region at $D \approx D_1+1$ which (since a_1 is the large

amplitude) may be the stable one in small changes of K_c. Of course, as we do not know what the amplitudes are, such a picture can only be justified a posteriori. One such example (for B=0.1 and U_0=0.05) is depicted in Figure (5.3), where for K_c=0.13098 there is a second convergence region around D ~ 1.75. Although the first convergence region in this plot is around D ~ 0.5 (and not D ~ 0.75, as it should be) one must recall that our original estimate for K_c=0.13088 gave an answer compatible with D ~ 0.75. Thus, although this scenario does not always work, it does sometimes improve our confidence limits (see Figure (5.4.a and b)). Note that the values of the analysis with a_0 dominance are considerably more inconsistent compared to the ones for which the dominant term was the a_1 term. This is true for both the γ and D_1 values.

It is now clear from Figure (5.4.a) that the confluent singularity analysis results in improved estimates for γ which, however, do not vary appreciably from those that were obtained with the simple D-log Pade analysis. This is probably true because the (admittedly poor) estimate for D_1 has always been a value close to one. Although we cannot conclude with confidence that our model has no confluent exponents, it is certain that if they are present, they do not compete appreciably with the dominant singularity.

Our full results are depicted on Table (5.1). It is clear that no significant universality restoration takes

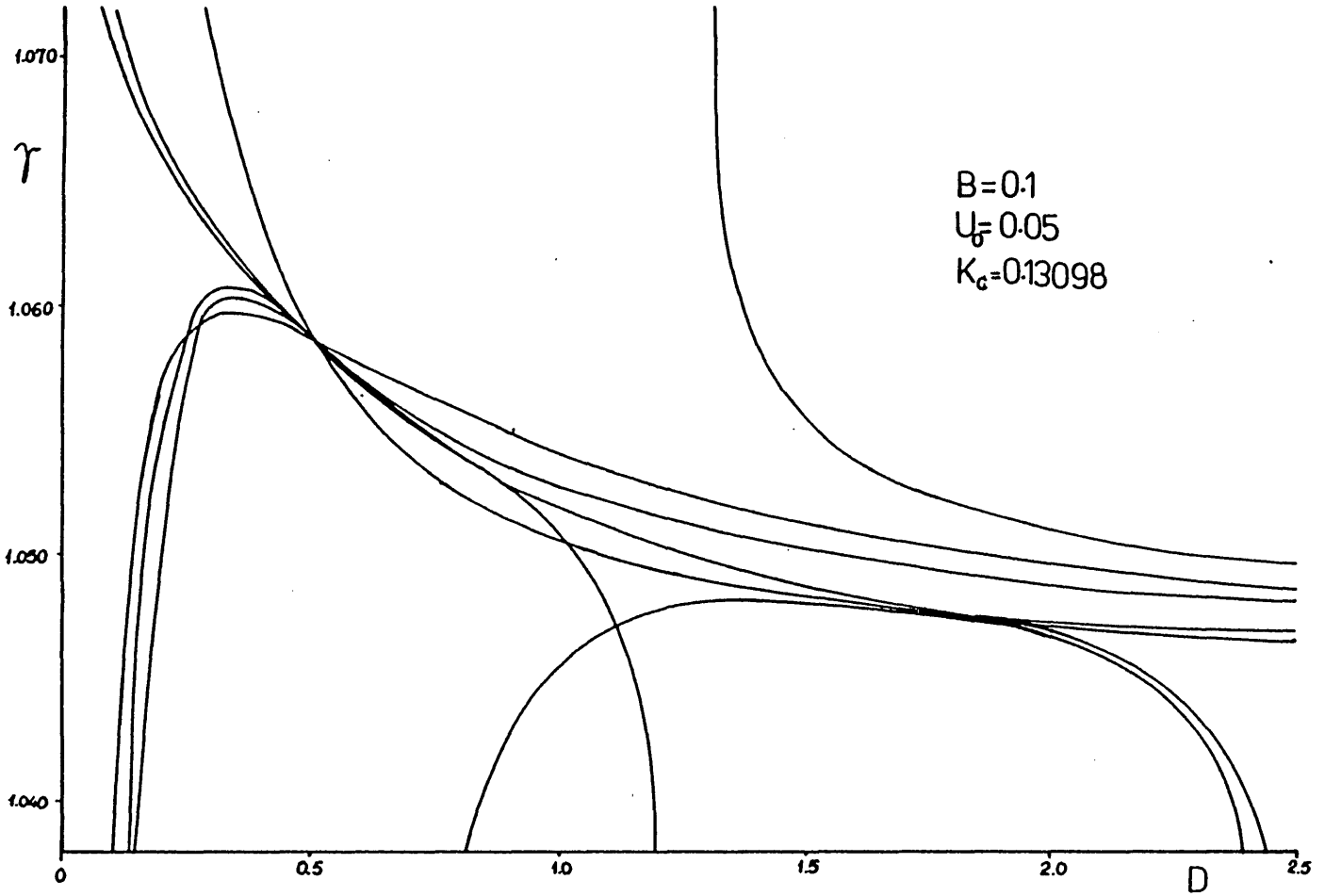


FIG. 5.3 : Same as Fig. 5.2 . There are two convergence regions.

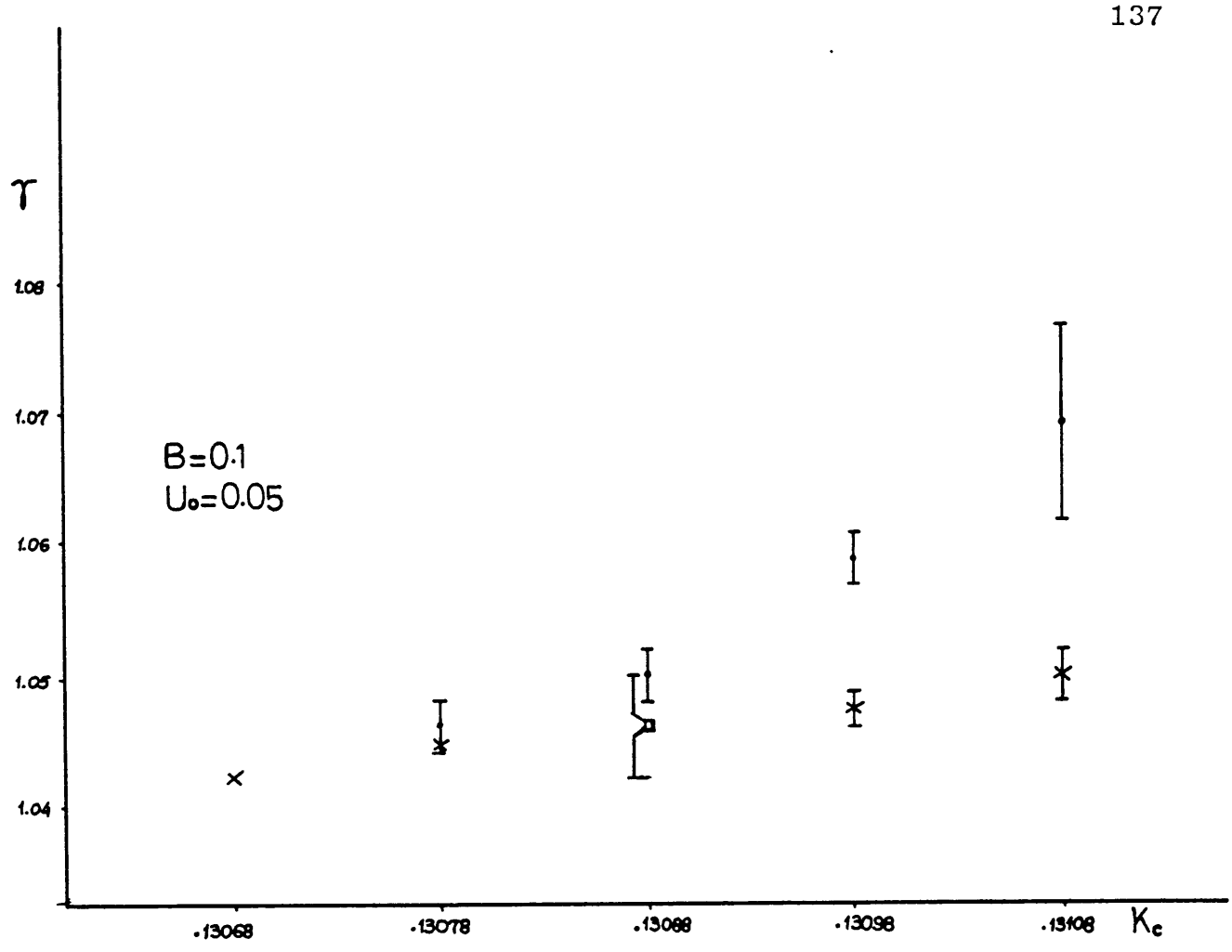


FIG. 5.4.a : Variation of γ estimates for different input values of K_c. Dots indicate results obtained from the first convergence region, crosses from the second.

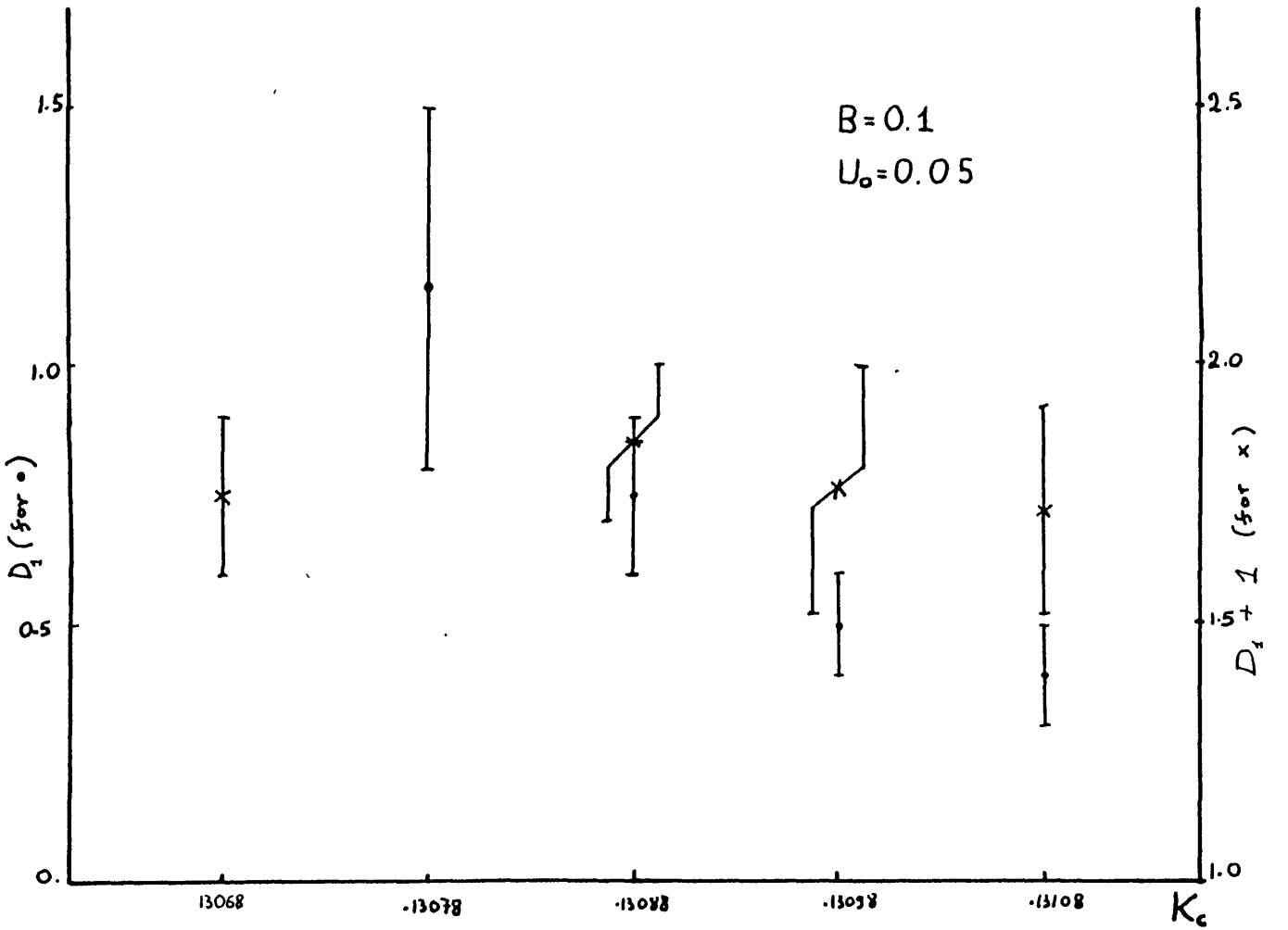


FIG. 5.4.b : Same as Fig. 5.4.a for the confluent singularity D_1.

Simple D-log Pade method				Adler et.al. method	
B	U_0	K_c	γ	γ	D_1
0.5	0.10	0.12875(0)	1.04(2)	1.0445(15)	0.98(14)
0.1	0.10	0.13393(0)	1.064(4)	1.0657(7)	0.89(11)
0.1	0.01	0.12560(1)	1.009(6)	1.0138(18)*	0.65(15)
0.1	0.05	0.13088(0)	1.046(4)	1.0506(18)	0.75(15)
0.3	0.15	0.13405(4)	1.066(4)	1.0689(7)	0.9(1)

Table 5.1 : Comparison of the results obtained with simple D-log Pade approximants to those obtained with the confluent singularity analysis of Adler et.al.

* This is the point closest to the tricritical region. The γ and D_1 values are unreliable. Note that they display the biggest variation from the mean of the measurements considered.

place. A look in Fig. (5.1) shows that all the points considered lie within the region where the model's single site spin distribution has one infinite peak ; thus even according to the weak universality notion of Baker and Johnson, the γ values within this region ought to be universal. Our results show a somewhat varying γ but, as we have argued in the previous Chapter, such small variations can be present near the tricritical region. Therefore as far as the universality hypothesis is concerned, our results are inconclusive but not incompatible with it.

In conclusion : (a) the new values of γ are trivially different from the old ones and (b) the new errors are an improvement on the old ones. This means that our analysis of Chapter III was done with the biggest possible errors. Had we repeated it fully, taking the influence of the confluent indices into account, we would have only succeded in narrowing the band of $\kappa=0$ points on the $B-U_0$ plane rather than shift it towards the tricritical area. Thus, our earlier neglect of confluent singularities has been justified, in that their presence does not alter our conclusions about the triviality of scale covariant $\lambda\phi^4$.

CONCLUSIONS

We examined a lattice field theory characterised by an action defined in a three dimensional real parameter subspace (K,B,U_o) with $B < 1$ and $U_o > 0$. We presuposed the existence of a critical surface in this subspace of the form $K_c = f(B, U_o)$, on which a second order phase transition occurs, thus enabling the lattice theory to have a continuum field theory limit on K_c. Neglecting any logarithmic critical behaviour near K_c, we managed to locate numerically a subsurface on which $\kappa = 0$, i.e. the theory is non-trivial. Using Monte Carlo simulations, we then scanned the region around this subsurface in order to justify our assumption that a continuum theory actually exists there. We found areas of both first and second order transitions on the critical surface. The $\kappa < 0$ region lies entirely within the first order transition area. The second order transition region is characterised by a $\kappa > 0$ behaviour. A confluent singularity analysis improved the errors without altering the main features of the theory. Thus, the theory is trivial. As a collorary, the canonical $\lambda\phi^4$ theory, lying on the $B = 0$ plane of the parameter space is found to be trivial.

PART B

INTRODUCTION

1. Generalities on lattice gauge theories and Monte Carlo simulations

In Part A of this thesis, we have examined a modified version of $\lambda\phi^4$ scalar field theory. In particular, we saw that the best way to have a good understanding of the model's behaviour and obtain reliable answers was to exploit its analogy to a well known Statistical Mechanical theory, the Ising model. Once the equivalence of scalar field theory to a statistical spin system in equilibrium was established, we could exploit all the existing techniques for studying spin systems in order to solve the model field theory.

This game is relatively old; since 1974 physicists have tried to use this similarity of spin systems to field theories as the standard alternative line of attack whenever perturbation theory failed. Not only field theoretic models (like $\lambda\phi^4$) but also the physical gauge theories have been intensively examined in the framework of a lattice regularisation. Given such a lattice formulation, a great number of different techniques, popular with solid state physicists, have been exploited in the study of gauge theories; these are both analytic (e.g. strong coupling expansions, mean field teory,

duality) and numerical (e.g. Monte Carlo simulations). Like Part A of this thesis, this considerably shorter second Part will deal with a field theory on the lattice. Unlike Part A, however, it will be a gauge theory, namely SU(2).

Although theories with gauge symmetry are of extreme physical importance nowdays, we are not going to deal, at least directly, with any problems related to the physics of SU(2) gauge theory. On the contrary, we shall be involved with a few technicalities that characterise the most popular method which is nowdays used to study lattice gauge theories, that of Monte Carlo (MC) simulations. In particular we shall see how the gauge fixing of the theory may influence the thermalisation properties and the statistics of a MC simulation. It is true that such aspects are of limited importance to the physics of gauge theories since they are problems related to the numerical techniques involved. However, MC simulations have lately developed into the major method of solving lattice gauge theories [73]. Their importance has lead to an unprecedented involvement of field theorists in games related to the improvement of numerical techniques, computer architecture and software development. Thus, our study of the effects of gauge fixing on MC simulations is carried out in this spirit.

Moreover, although we have been unable to give a definite explanation of our numerical results, a plausibility argument is briefly presented at the end.

This is of some interest, since it relates MC thermalisation phenomena to non-equilibrium Statistical Mechanics. Although we have been unable to utilise it, the connection is there.

CHAPTER VI

GAUGE FIXING AND MONTE CARLO SIMULATIONS

1. Formulation of gauge theories on the lattice

Gauge theories on the lattice have been proposed by Wilson [74]. The essential idea is to make the theory as well defined as possible (by regularising it on a lattice) even at the cost of loosing Lorentz invariance, while, however, preserving the all important gauge invariance. The way to achieve this was not straightforward; Wilson has found out that in order to be consistent with such a scheme, he had to set up the whole theory from scratch (i.e. arbitrarily define what the fundamental degrees of freedom, action and gauge theory are, rather than deduce them from analogies to the known continuum physics). In particular, one must give up the notion that the fundamental degrees of freedom are the gauge fields $A_\mu(x)$ which are elements of the gauge algebra; in the lattice formulation of pure gauge theories, we define the dynamical variables to be elements of the gauge group which are associated with each bond of the lattice. Since an oriented bond can be completely defined by a site k and a direction μ, the dynamical variables are anotated by

$$G_b \equiv G_\mu(k) \equiv \exp(iag\, A_\mu(k)) \tag{6.1}$$

where $A_\mu(k) \equiv A_\mu(x)$ is the gauge field, a is the lattice spacing ($x \equiv ak$) and g is the theory's coupling constant. We then define gauge group elements g(k) which live on the lattice sites and are not dynamical degrees of freedom; they are only there in order to gauge-transform the dynamical variables according to the following gauge transformation

$$G_\mu(k) \rightarrow G_\mu(k)' = g(k)\, G_\mu(k)\, g(k+\mu)^{-1} \tag{6.2}$$

Finally, Wilson [74] proposed the plaquette action. For each plaquette, which may be labeled by a site k and two directions μ and ν, we have an elementary action

$$S_p \equiv S_{\mu\nu}(k) \equiv 1 - \tfrac{1}{2}\, \mathrm{ReTr}[G_\mu(k)\, G_\nu(k+\mu)\, G(k+\nu)^{-1}\, G_\nu(k)^{-1}] \tag{6.3}$$

for an SU(2) pure gauge theory. the total action is simply the sum of the plaquette action over all plaquettes, i.e.

$$S = \sum_p S_p \tag{6.4}$$

The theory's generating functional is defined to be

$$Z = \int \prod_b dG_b \quad \exp[-\beta\, S(G_p)] \tag{6.5}$$

where dU_b is the gauge invariant Haar measure [38] and

$$\beta \equiv 4 \,/\, g^2 \tag{6.6}$$

is the inverse coupling constant. Starting with the action (6.3) and with the aid of definitions (6.1) and (6.6) the action for the lattice pure gauge theory reduces to the continuum Yang Mills action (see [74] and also the reviews [38,39])

Now the typical lattice gauge invariant correlation function which is interesting to study is the Wilson loop; i.e. a product of oriented link group elements which belong to a closed contour C of the lattice:

$$< W(C) > = \int \prod_b dG_b \quad W(C)\, \exp(-\beta S) \tag{6.7}$$

where

$$W(C) \equiv Tr \left(\prod_{b \in C} G'_b \right) \tag{6.8}$$

The simplest Wilson loop consists of the boundary of an elementary lattice plaquette. Provided we also average over all such plaquette contours on the lattice, this object is known as the "average plaquette".

In order to study this lattice version of the gauge theory, we will use a suitable parametrisation of the dynamical variables which was proposed by Creutz [73]. He pointed out that SU(2) group elements can be parametrised in the form

$$G = a_o I + \underline{a}\,\underline{\tau} \qquad (6.9.a)$$

where $a_\mu \equiv (a_o, \underline{a})$ is a four vector of unit length

$$a_o^2 + \underline{a}^2 = 1 \qquad (6.9.b)$$

I is the 2X2 unit matrix and $\underline{\tau}$ are the three Pauli matrices. The invariant Haar measure is then given by

$$dG = \frac{1}{2\pi^2}\ \delta(a^2-1)\ d^4a \qquad (6.9.c)$$

As we shall see in Section 3, this parametrisation is extremely useful for MC simulations.

2. Gauge fixing on the lattice.

Just like for the $\lambda\phi^4$ model of Part A, once our gauge theory is put on the lattice, it becomes a perfectly well defined theory. As is suggested by eqn. (6.5), the generating functional is a multiple integral which, for a finite size lattice consists of a finite

number of definite integrals. Since the integration is over the group (rather than the algebra) space, and since the group is compact, nothing is ill defined. This is to be contrasted to the case of continuum physics, where the gauge symmetry renders the integrations over the algebra space infinite unless we introduce the Fadeev-Popov ghost term in the action [3]. In the lattice formulation of gauge theories, counterterms and ghost terms are unnecessary.

On the other hand, we have the freedom to eliminate a few degrees of freedom. This can be done by gauge fixing. In particular, one may use a judicious choise of the site SU(2) elements g(k) to fix a number of links to the value of a constant group element (say, the unit element of the group). Thus, a g(k) and a g(k+μ) can be found such that (6.2) becomes

$$G_\mu(k) \rightarrow G_\mu(k)' \equiv 1 \qquad (6.10)$$

This means that the corresponding algebra element $A_\mu(k)$ is fixed to zero. This process may be repeated for more lattice links until a point is reached when all the site group elements have been used up to fix gauge degrees of freedom. In such a case, the gauge fixing is maximal.

A few applications of this process will illuminate the situation. In Figure (6.1) a maximal gauge fixing has been performed for a two dimensional finite size (4X4) lattice with free boundary conditions. In (a), the

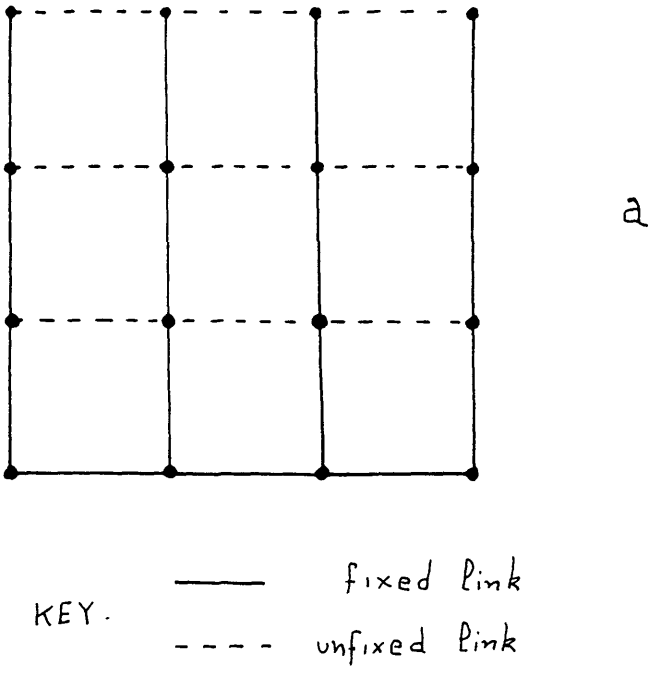


FIG. (6.1) : Gauge fixing on a 4X4 lattice with free boundary conditions
(a) maximal axial gauge
(b) maximal random tree gauge

gauge fixing is axial, in that all links in one direction are fixed. Note that maximal gauge fixing allows us to freeze a few extra degrees of freedom of the system in another direction as well; this was not so for the axial gauge in the continuum. In (b), the same process was repeated, but no special care has been taken to fix the links of one particular direction; this gauge fixing we shall term random tree gauge.

The same ideas can be applied when the lattice has periodic boundary conditions. Now, the two dimensional lattice is a torus. It is depicted in Figure (6.2). Gauge fixing is almost the same; the only difference being that the links which, because of the periodic boundary conditions, "curve back" to the lattice edges, have to be unfixed. Thus, the axial gauge is incomplete.

The whole situation can be generalised in d dimensions [75,76]. Given a hypercubic lattice of size $a_1 x a_2 x \ldots x a_d \equiv V$ with periodic boundary conditions, denote any lattice point n by a set of d integers $(n_1, n_2, \ldots, n_d)$ with $1 \leq n_\mu \leq a_\mu$. We may fix all dynamical variables to unity on a maximal tree which consists of a set of V-1 links and satisfies the properties: (a) it visits all points on the lattice (b) it contains no closed loops and (c) it leaves one gauge transformation undetermined. For the special case of the axial gauge this means that the gauge fixing is the following:

$U_d(n) = 1$ for all n with $n_d \leq a_d - 1$

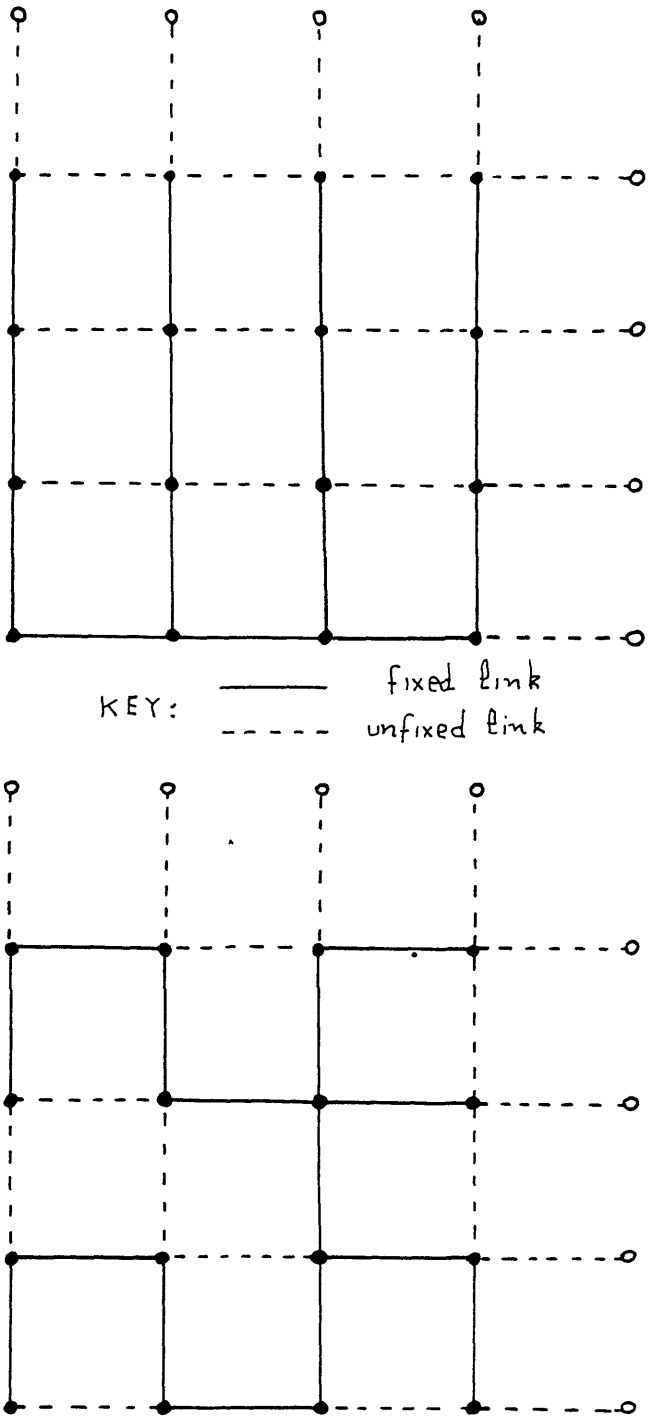


FIG. (6.2) : Same as (6.1) but for a lattice with periodic boundary conditions The "open circle" edge sites at the top and on the right coincide with the edge sites at the bottom and on the left.

$U_{d-1}(n)=1$ for all n with $n_d=1$, $n_{d-1}<a_{d-1}-1$

$U_1(n)=1$ for all n with $n_d=n_{d-1}=\ldots=n_2=1$, $n_1<a_1-1$

3. Monte Carlo theory

At the time of writting, MC simulations are considered as the most powerful numerical method of solving Euclidean lattice regularised field theories. It is the only promising method of a direct calculation of such a fundamental non-perturbative problem as the QCD mass spectrum. Thus, we shall devote this Section to a brief description of the method.

The MC method is used to make approximate calculations of integrals by summing over randomly selected points in the integration domain. In field theories, it is applied to the calculation of operators like

$$\langle f \rangle = \int dU_b \; f[U_b] \exp(-\beta S(U_p)) \qquad (6.11)$$

where the operator $f(u_b)$ is a functional of a lattice field configuration $\{U_b\}$. The essence of the method is the following: The computer is used to generate lattice configurations one after the other; we denote by τ the discrete computer time (we will sometimes refer to it as "fifth time") in the course of which these configurations are generated in a step by step fashion. Two probability notions are important: (a) the normalised transition

probability p_{ij} of jumping from configuration $\{U_b(i)\}$ to the state $\{U_b(j)\}$ in one computer τ-time step τ and (b) the normalised probability of each configuration which for systems in thermal equilibrium is given by the Boltzman distribution

$$\pi_j \equiv \pi(U(j)) = Z^{-1} \exp(-\beta S) \qquad (6.12)$$

(we have dropped the subscript b from the bond element)

The essence of the MC method is to approximate expectation values like the one of eqn. (6.11) by a sum

$$Y(\tau) = \frac{1}{\tau} \sum_{i=1}^{\tau} f[U(i)] \qquad (6.13)$$

We will avoid any details which involve otherwise irrelevant topics such as Markov chains; the reader is referred to [77,38] for a lenghtier treatment of MC theory. Here we shall only state that such an approximation is justified by a theorem which states that

$$Y(\tau) - \int dU\ \pi(U)\ f(U) \sim O(1/\sqrt{\tau}) \qquad (6.14)$$

which renders the approximation reliable for large τ. One only needs to generate in the computer τ number of appropriate lattice configurations and then calculate $f[U(\tau)]$ and $Y(\tau)$ explicitly. For large τ, $Y(\tau)$ will

converge to the desired expectation value $\langle f(U) \rangle$.

It is now quite clear that the method is expected to work at least in principle but also in practice, provided that it is possible to generate configurations $\{U(i)\}$ at each "fifth time" step i, with the probability distribution of eqn. (6.12). This is known as importance sampling and it can be achieved in two ways: (a) the Metropolis et. al. algorithm [58] and (b) the heat bath algorithm. These are now briefly described.

The Metropolis et. al. algorithm involves a generation of states with an initialy arbitrary normalised symmetric transition probability p^*_{ij}. This leaves us the freedom, once we have an inital lattice configuration $\{U(i)\}$, to generate the next one $\{U(j)\}$ almost arbitrarily. We then define the transition probability

$$p_{ij} = \begin{cases} p^*_{ij} \, \pi_j/\pi_i & \text{if } \pi_j/\pi_i < 1 \\ p^*_{ij} & \text{if } \pi_j/\pi_i > 1 \end{cases} \qquad (6.15)$$

Recall that

$$\pi_j/\pi_i \propto \exp(-\beta \, \Delta S) \qquad (6.16.a)$$

with

$$\Delta S = S(U(j)) - S(U(i)) \qquad (6.16.b)$$

Since it turns out that p_{ij} satisfies all the requirements of Markov chain theory for which eqn. (6.14) is valid [77], all that we need to do is ensure that the computer updates configurations, calculates the change in the action ΔS and accepts or rejects the update with criterion (6.15). A significant detail of the theory is that the requirement known as detailed balance condition

$$\pi_i \, p_{ij} = \pi_j \, p_{ji} \tag{6.17}$$

is satisfied.

Unlike the Metropolis et.al. algorithm, which can be applied to any lattice action $S[U_p]$, the heat bath algorithm [73] depends on the particular symmetry group we are dealing with. The idea is to generate new configurations by successively touching a heat bath to each link variable. Each link element U is replaced by a new one U', chosen randomly with probability density proportional to the Boltzman factor

$$dP(U') \propto \exp[-\beta \, S(U')] \, dU' \tag{6.18}$$

In order to generate this probability density, we consider the SU(2) parametrisation given in eqns. (6.9). The part of the theory's action which contributes to exponentials like that of eqn. (6.18) is the contribution

of the six plaquettes touching the link U; thus we may write

$$dP(U) = dP(U)\, \exp\left[\tfrac{1}{2}\, \beta\, \mathrm{Tr}\left(U \sum_{\alpha=1}^{6} \tilde{U}_\alpha\right)\right] \qquad (6.19)$$

where by $\tilde{U}_\alpha$ we denote the six products of the link variables which interact with the link in question. The useful property of SU(2) elements is that

$$\sum_{\alpha=1}^{6} \tilde{U}_\alpha = k\bar{U} \qquad (6.20.a)$$

where $\bar{U}$ is an SU(2) element and

$$k^2 = \det\left(\sum_{\alpha=1}^{6} \tilde{U}\right) \qquad (6.20.b)$$

The next step is to use the invariance of the group measure [38] to write

$$dP(U\,\bar{U}^{-1}) \propto dU\, \exp\left[\tfrac{1}{2}\, \beta\, k\, (\mathrm{Tr}U)\right] = \frac{1}{2\pi^2}\, \delta(a^2-1)\, e^{\beta k a_o}\, d^4a \qquad (6.21)$$

If we choose the new link element to be $U' = U\,\bar{U}^{-1}$, we see that all we need is to generate a probability density according to (6.21). This can be done easily, as it only involves randomly generating points on the surface of a four dimensional unit sphere with exponential weighting

along the a_o direction [73].

4. Gauge fixing and Monte Carlo relaxation

We have repeatedly stressed that MC simulations have recently become very important in the study of hadronic physics. In the course of this development, more and more computer resources are required. This is necessary for obtaining results for more complicated physical quantities, on bigger lattices, with improved statistical error analysis. Thus, one is tempted to improve the basic MC methods in order to gain in numerical reliability.

One possible line of approach is the effort to exploit the gauge symmetry of the theory in order to achieve faster thermalisation and improved statistics. In particular, as we explained in Section 2, one is free to "freeze" about one quarter of the lattice link variables to a constant value. This is just the result of fixing the gauge of the theory; apart from this the theory is the same and MC simulations can be carried out as before. The possible gain, however, is that MC runs with the new action will not involve the systematic updating of all the lattice links but only those which are not gauge fixed. Thus, if all the other things are to remain the same, one naively expects to obtain the same answers with less computing. (We found out that typical gains in computer time ranged between 5% and 10%,

a significant amount.) Unfortunately, other things do not remain the same. In his seminal MC paper [73], Creutz had hinted that in the study of SU(2) theory, once the axial gauge is chosen, the relaxation from different initial configurations to equlibrium is slower than without gauge fixing. As he never presented any results, we looked into the matter more carefully. We must emphasise that Creutz's results were based on runs which are very slow by today's standards. Typical measurements of the average plaquette were performed with only 30 to 50 iterations; thermalisation was regarded adequate after 10 to 15 iterations.

Thus, we investigated the problem carefully by performing a few hundred iterations on a 4^4 lattice with periodic boundary conditions, using both hot and cold starts. We used the heat bath algorithm of Creutz. Our results consist of computing the average plaquette in three cases: (a) without fixing the gauge, (b) with an axial gauge and (c) with a random tree gauge. For the axial gauge the links can be fixed in the standard directional pattern. For the random tree gauge, a program had to be written according to which, starting from a particlar site, we navigate randomly through the lattice, fixing links according to the requirements of Section 2 (no loops etc) until a maximal tree has been created. About a quarter of the total number of fixed links correspond to each space time direction. This tree has been formed once and for all; then this information

is stored and used as input for subsequent MC runs.

We performed simulations for nine different values of the inverse coupling β. We present those results which are most representative of the different characteristic behaviour of SU(2) lattice gauge theory. As is well known [73], the theory has a strong- and a weak- coupling region, separated smoothly by a crossover region at about $\beta=2.2$. The crossover region is due to a neighbouring phase transition on the extended SU(2)-SO(3) real parameter space [78].

In Figure (6.3) we show our results at $\beta=2.2$. It is clear that without gauge fixing, thermalisation is faster. The random tree gauge is better than the axial. Similar behaviour was observed for $\beta=2.0$ and $\beta=1.2$, although in the last case the difference in behaviour between the three gauges was less vigorous. Indeed, as β is further decreased (high temperature regime) thermalisation is faster in all three cases and none of them is significantly better than the other. We have seen this for $\beta=0.9$ and $\beta=0.1$ (the last case is shown in Figure (6.4)).

This behaviour is no surprise. According to eqns. (6.12) and (6.18), when $\beta \to 0$, the probability distribution becomes unity; i.e. all configurations of the canonical ensemble contribute equiprobably. Thus, since they are all accepted by MC trials, the sampling proceedure (with or without gauge fixing) becomes unimportant.

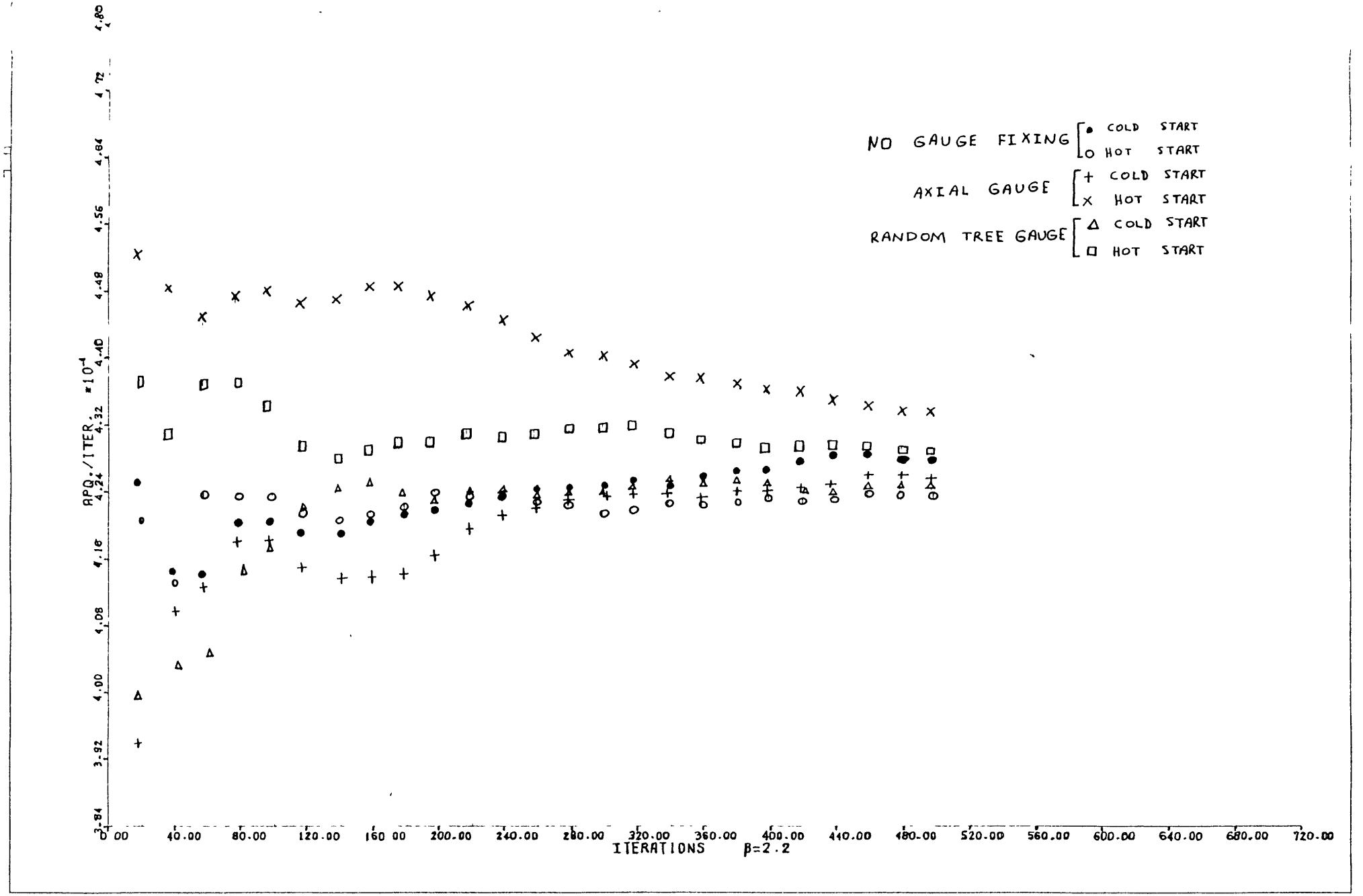


FIG. (6.3) : Relaxation to equilibrium at $\beta = 2.2$

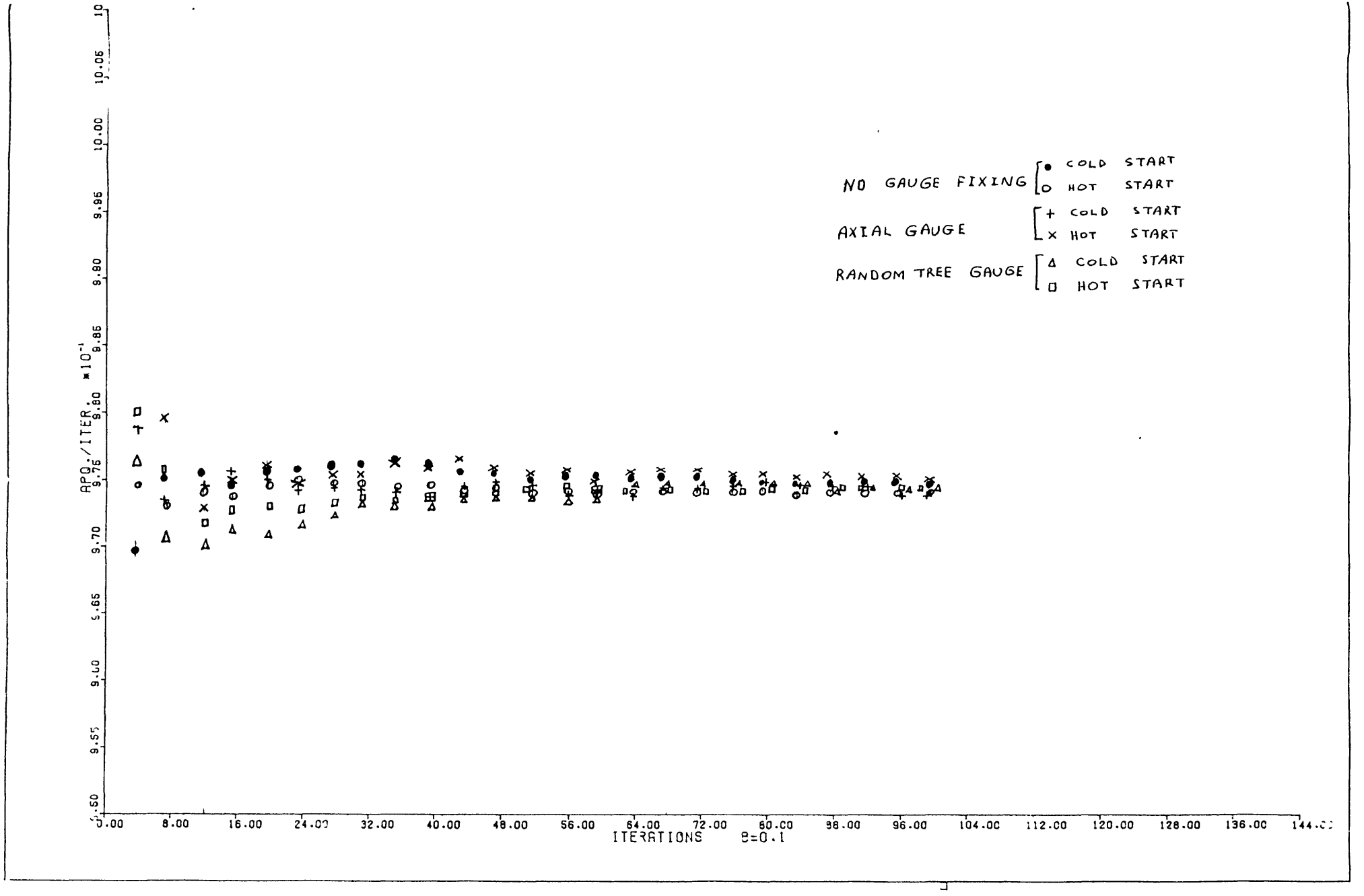


FIG (6.4) : Relaxation to equilibrium at $\beta = 0.1$

On the other hand, if we start looking at weaker couplings, thermalisation without gauge fixing is always the fastest of the three. In some cases (β=2.6, β=5.1) the axial gauge converges marginally faster than the random tree gauge; in others (β=3.2) the situation is reversed and sometimes they behave almost identically (β=9.5). This last case is shown in Figure (6.5).

This weak coupling behaviour is quite surprising and counter-intuitive. We know from the behaviour of the Boltzman distribution (eqn. (6.12)) that as $\beta \to \infty$, only the configurations which minimise the action S will contribute. Given the definition of the action (eqn. (6.3)), it is evident that for large β, the only surviving configurations are those for which the bond variables equal or nearly equal the unit group element. Thus, at large β one would naively expect that gauge fixing, which already fixes about a quarter of the links to the desired value, would somehow help the system attain equilibrium faster. This is unfortunately not so.

In all cases, Creutz's conclusion was verified, despite the increased number of iterations and the implementation of an asymetric (axial) and a symmetric (random tree) gauge: when the gauge is fixed, the lattice takes longer to arrive at thermal equilibrium. We have no explanation to offer for this behaviour. A handwavy attempt to an interpretation of this phenomenon will be given with the final conclusions.

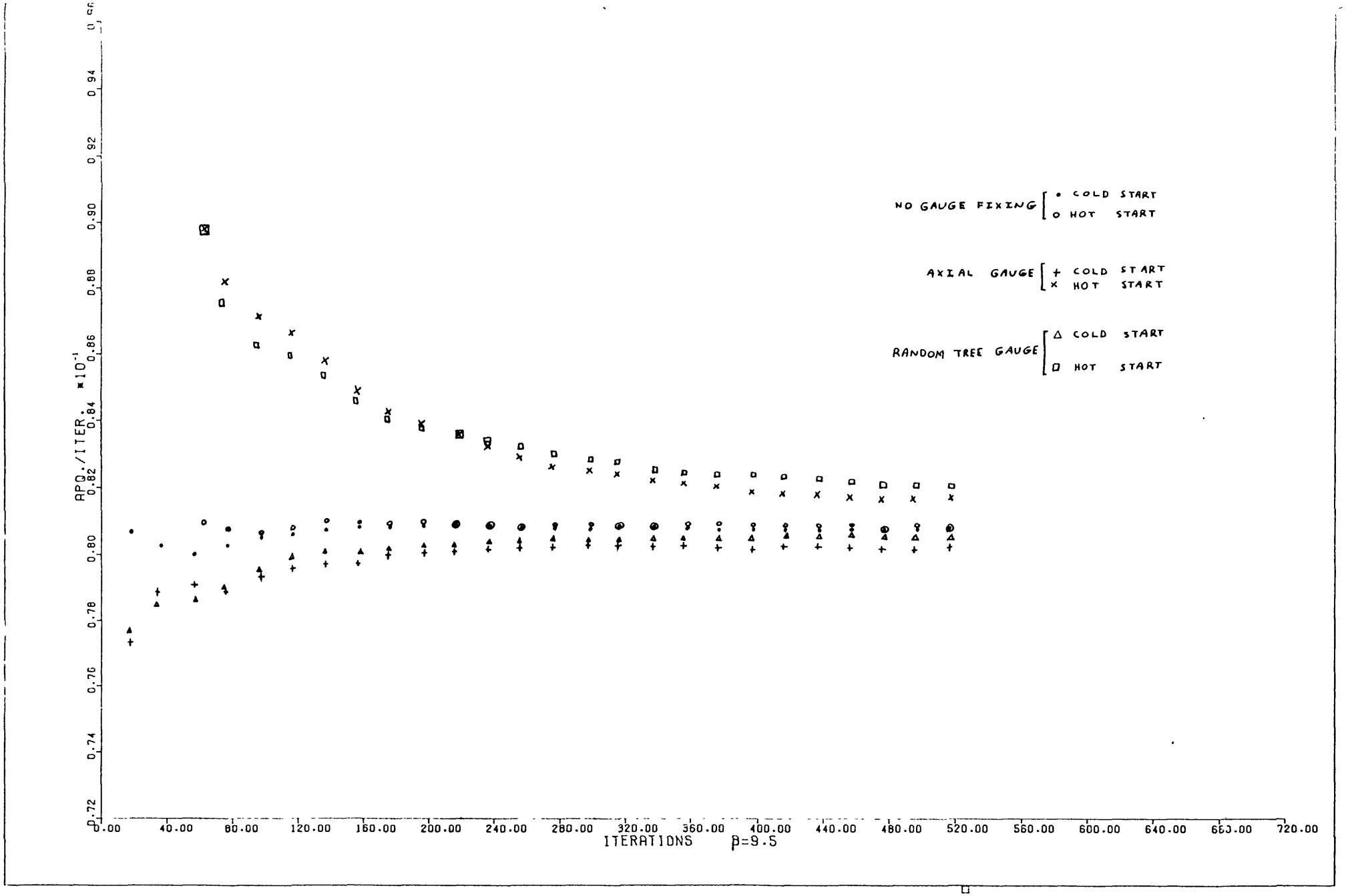


FIG (6.5) : Relaxation to equilibrium at $\beta = 9.5$

5. Gauge fixing and error analysis

So far we have dealt with the effects of gauge fixing on the convergence to equilibrium problem. We will now turn our attention to a more important aspect of this game, namely that of error analysis. We know that the error of a MC estimate is given by the ratio

$$\delta A = \sigma / \sqrt{\tau} \qquad (6.22)$$

where σ is the standard deviation of our measurements

$$\sigma \equiv \langle A^2 \rangle - \langle A \rangle^2 \qquad (6.23)$$

and τ the number of iterations. Here A stands for the measured quantity (the average plaquette) and $\langle A \rangle$ for the mean of A over the number of τ measurements.

This is a standard result [59] but only if we assume that the measurements are uncorrelated. This assumption is unjustified, since in practical MC programs the Markov chain is generated from the previous one by only a small change. Thus, the presence of correlations between measurements is guaranteed. Correlations are a source of underestimation of MC errors and thus a permanent headache. The standard way to tackle this problem is an empirical one: One may safely assume that correlations are strong between adjacent measurements but largely separated measurements are virtually uncorrelated.

There are two ways to exploit this idea. Both ways involve a proceedure of "blocking" the measurements in small groups; i.e. having performed a number of measurements, we split up their total in groups of N adjacent measurements which we will call blocks. Denote by M the number of blocks, so that the total number of measurements is MXN. Now the first method relies on the fact that if we work out the mean value of the measurements of each block, and denote by σ_1 the standard deviation of these means, this is related to the standard deviation σ of eqn. (6.23) by

$$\delta A = \sigma^2 / MN = \sigma_1^2 / M \qquad (6.24)$$

provided that the measurements are uncorrelated. So, if the measurements were uncorrelated, the error δA should be the same irrespective of whether we block or not. Departure from this behaviour gives a measure of correlations. This we term Method 1.

We will now describe Method 2. It is a simple variant of the method proposed in [59]. From each block of size M, we drop the first N-1 measurements and consider just the Nth. Thus, we have a total of M measurements, with standard deviation σ_2 and error $\delta A_2 = \sigma_2 / \sqrt{M}$. Provided we do not have any correlations, this error is related to the original error of eqn. (6.22) by

$$\delta A = \delta A_2 / \sqrt{N} \qquad (6.25)$$

Deviation from this relationship measures the presence of correlations. Although we have used both methods, we believe that Method 1 is somewhat more reliable, because it uses all the available information (i.e. it does not throw any measurements away).

We have used the two methods in order to compare the reliability of the errors with and without gauge fixing. Typical results are shown in Table (6.1) and (6.2). Each column is labeled by the size of the blocks. The abbreviation M1(C) stands for "results obtained with Method 1 and cold starts"; analogously for M1(H), M2(C), M2(H). Also note that columns labeled APQ are the measurements of the average plaquette and those labeled δA are the corresponding errors. The figures in bracketts are the quantity $\delta A_2/\sqrt{N}$ of (6.25) which is used for the criterion of Method 2. These measurements were obtained over 1000 iterations, the first 100 of which were dropped, in order to let the system thermalise.

In an ideal situation without correlations, the errors from Method 1 and the figures in bracketts from Method 2 should agree reasonably well across each horizontal line of the Tables. We see that this is indeed the case from the results of Method 2. No significant fluctuations between the errors are observed. From Method 1, however, we see that significant

NO GAUGE FIXING

SIZE OF BLOCKS	1		5		10		15		20		25	
	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A
M1(C)	.42612	.00052	.42612	.00100	.42612	.00124	.42612	.00141	.42612	.00143	.42612	.00142
M2(C)	.42612	.00052	.42514	.00108 (.00048)	.42469	.00150 (.00048)	.42495	.00202 (.00052)	.42551	.00220 (.00049)	.42380	.00218 (.00044)
M1(H)	.42881	.00049	.42881	.00092	.42881	.00110	.42881	.00128	.42881	.00134	.42881	.00142
M2(H)	.42881	.00049	.42856	.00108 (.00048)	.42921	.00161 (.00051)	.42858	.00201 (.00052)	.42916	.00268 (.00060)	.42732	.00243 (.00049)

AXIAL GAUGE

SIZE OF BLOCKS	1		5		10		15		20		25	
	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A
M1(C)	.42148	.00051	.42148	.00100	.42148	.00132	.42148	.00154	.42148	.00172	.42148	.00184
M2(C)	.42148	.00051	.42199	.00117 (.00052)	.42154	.00158 (.00050)	.42362	.00196 (.00051)	.42272	.00237 (.00053)	.42359	.00268 (.00054)
M1(H)	.42983	.00051	.42983	.00101	.42983	.00133	.42983	.00157	.42983	.00172	.42983	.00184
M2(H)	.42983	.00051	.42945	.00110 (.00049)	.42927	.00161 (.00051)	.42777	.00177 (.00046)	.42819	.00232 (.00052)	.42979	.00261 (.00052)

RANDOM TREE GAUGE

SIZE OF BLOCKS	1		5		10		15		20		25	
	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A	APQ	σ_A
M1(C)	.42752	.00050	.42752	.00096	.42752	.00125	.42752	.00147	.42752	.00160	.42752	.00169
M2(C)	.42752	.00050	.42729	.00113 (.00051)	.42664	.00156 (.00049)	.42699	.00202 (.00052)	.42758	.00228 (.00051)	.42938	.00234 (.00047)
M1(H)	.42788	.00044	.42788	.00084	.42788	.00107	.42788	.00118	.42788	.00132	.42788	.00136
M2(H)	.42788	.00044	.42808	.00097 (.00043)	.42859	.00139 (.00044)	.42892	.00162 (.00042)	.42769	.00204 (.00046)	.43068	.00198 (.00040)

TABLE (6.1) : Error analysis for β=2.2

NO GAUGE FIXING

SIZE OF BLOCKS	1		5		10		15		20		25	
	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$
M1(C)	.08076	.00006	.08076	.00008	.08076	.00008	.08076	.00008	.08076	.00008	.08076	.00009
M2(C)	.08076	.00006	.08062	.00012 (.00006)	.08074	.00018 (.00006)	.08074	.00021 (.00005)	.08047	.00026 (.00006)	.08037	.00029 (.00006)
M1(H)	.08067	.00006	.08067	.00007	.08067	.00008	.08067	.00007	.08067	.00007	.08067	.00008
M2(H)	.08067	.00006	.08054	.00014 (.00006)	.08050	.00018 (.00006)	.08074	.00025 (.00006)	.08035	.00026 (.00006)	.08065	.00037 (.00007)

AXIAL GAUGE

SIZE OF BLOCKS	1		5		10		15		20		25	
	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$
M1(C)	.08053	.00006	.08053	.00008	.08053	.00009	.08053	.00010	.08053	.00011	.08053	.00010
M2(C)	.08053	.00006	.08037	.00013 (.00006)	.08017	.00019 (.00006)	.08014	.00021 (.00005)	.08046	.00026 (.00006)	.08082	.00028 (.00006)
M1(H)	.08093	.00007	.08093	.00011	.08093	.00013	.08093	.00015	.08093	.00015	.08093	.00016
M2(H)	.08093	.00007	.08087	.00016 (.00007)	.08061	.00023 (.00007)	.08112	.00027 (.00007)	.08034	.00030 (.00007)	.08071	.00041 (.00008)

RANDOM TREE GAUGE

SIZE OF BLOCKS	1		5		10		15		20		25	
	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$	APQ	$\sqrt{A}$
	.08069	.00006	.08069	.00008	.08069	.00010	.08069	.00010	.08069	.00012	.08069	.00012
	.08069	.00006	.08066	.00014 (.00006)	.08063	.00019 (.00006)	.08043	.00023 (.00006)	.08078	.00026 (.00006)	.08089	.00029 (.00006)
	.08143	.00007	.08143	.00010	.08143	.00012	.08143	.00014	.08143	.00014	.08143	.00015
	.08143	.00007	.08136	.00015 (.00007)	.08120	.00021 (.00007)	.08149	.00020 (.00005)	.08113	.00030 (.00007)	.08120	.00032 (.00006)

TABLE (6.2) : Error analysis for $\beta = 9.5$

fluctuations between the errors occur, for different sizes of blocks. As this method is more reliable, this is a signal that correlations are actually present. A glance at the Tables shows that they appear to be marginally stronger for the gauge fixed case. Given this, we conclude that no significant benefit will arise from a computational point of view by fixing the gauge. Although not considerably, the errors were worse than without gauge fixing.

CONCLUSIONS AND DISCUSSION

We have seen that gauge fixing, contrary to naive expectations, does not seem to improve the quality of MC simulations. Although, once the gauge is fixed, as a result of fewer link updates, the same number of lattice sweeps occur in less CPU time, convergence to equilibrium is slower and the errors are longer. Correlations also seem to persist marginally longer. We were unable to give any reasonable explanation of all this. There is, however, a plausibility scenario which can at least give a better understanding to the thermålisation effect. We stress that it is only a proposition which sounds plausible but for which no proof can be given. This is why we will discuss it as briefly as possible.

The argument is based on the idea of Stochastic Quantisation as proposed by Parisi and Wu [79]. They assigned to the fields U of any quantum theory an extra dependence on a "fifth time" τ (i.e. $U=U(x_\mu, \tau)$) and postulated that the field obeys a particular Langevin equation. A standard result of non equilibrium Statistical Mechanics [80] is that if the field obeys a Langevin equation, the probability distribution $P(U,\tau)$ of the field obeys the so-called Fokker-Planck equation which in turn can be written as a Schrodinger eigenvalue equation

$$2\,H\,\phi \;=\; -\,\frac{\partial\phi}{\partial\tau}$$

where

$$H = \int d^4x \,\{\, \frac{\delta^2}{\delta U^2} + \frac{\delta}{\delta U}\,(P\,\frac{\delta S}{\delta U})\,\}$$

and

$$\phi \;= P\,\exp(S/2)$$

Here $S[U]$ is the theory's action. The result of interest for us is that for large "times" ($\tau \to \infty$) this probability behaves like

$$P \propto \exp(-S) + O(\exp(-2\lambda\tau))$$

where λ is the mass gap of H (i.e. its first eigenvalue). Thus, P tends to the Boltzman probability distribution of thermal equilibrium.

The relavance of all this is obvious. If the "fifth time" τ of this formalism can be identified with the MC computer time, the last equation states that the probability distribution relaxes to its equilibrium state with typical relaxation times

$$\tau \sim 1/\lambda$$

where λ is the first eigenvalue of H. Now H is gauge dependent, so in principle its spectrum ought to depend on the choise of gauge. If, when fixing the gauge, λ decreases, then the relaxation time becomes longer. Thus, the observations of the previous Chapter could be interpreted.

The problem with this approach is that the Fokker-Planck Hamiltonian is a very complicated object. Consequently, it does not seem possible to evaluate its spectrum. Therefore, although this whole picture seems plausible enough, it has not been proved to be true. One recent result which has strengthened our belief in this picture is that of Lautrup [81]. He managed to show that at least for the simple case of an action consisting only of a potential which depends on a scalar field $V(\phi(x))$, the Fokker-Planck formalism is equivalent to the detailed balance condition (eqn. (6.17)). Thus, the formalism of Stochastic Quantisation appears to be a Markovian process of the MC type, and our conjectures concerning the reasons of the particular behaviour that governs MC relaxation are reinforced.

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