

**A CROSSOVER SCALING STUDY OF THE
QUASI-TWO-DIMENSIONAL ISING MODELS**

ABSTRACT

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**DEPARTMENT OF PHYSICS
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**SUBMITTED IN FULFILMENT OF THE REQUIREMENT OF
THE DEGREE OF DOCTOR OF PHILOSOPHY**

To



**THE NORTH-EASTERN HILL UNIVERSITY
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I certify that the thesis entitled " A Crossover Scaling Study of the Quasi-two-dimensional Ising Models ", submitted by Miss Wendy Loslet Basaiawmoit for the Degree of Doctor of Philosophy of the North-Eastern Hill University, Shillong embodies the record of original investigation carried out by her under my supervision. She has been duly registered and the thesis presented is worthy of being considered for the Award of the Ph.D. Degree. This work has not been submitted for any Degree of any other University.

Date : 10th January, 1983.

Surjit Singh
Signature of the Supervisor

Place : Shillong.

ABSTRACT

Quasi-two-dimensional models have been of recent experimental and theoretical interest (1,2). These are really three-dimensional, but the interactions in the off-plane directions are much weaker than the intraplanar bonds. The crucial parameter determining the critical behaviour of such a system is g , the ratio of the two types of interactions. For relatively large values of g , say $\gtrsim 10^{-2}$, the system shows a three-dimensional behaviour. In this case, standard Padé approximant methods can be used to describe the system for the whole temperature range. On the other hand, if g is smaller, the system shows the true three-dimensional behaviour only on approaching the critical temperature very closely. If one moves away from the critical temperature, one sees a crossover to the two-dimensional behaviour for a range of temperatures. This can be described nicely in terms of the crossover scaling theory of Riedel and Wegner (3) as extended by Pfeuty, Fisher and Jasnov (4).

The aim of this dissertation was two-fold. Firstly, it was proposed to check the predictions of the crossover scaling theory in detail using the high-temperature series expansions. The second aim was to construct accurate approximants for thermodynamic quantities valid within the critical region. It was decided to restrict this study to the ordering susceptibility because, being the most singular thermodynamic quantity, it is highly suitable for studying the critical behaviour. Also, the information gotten from this about critical temperatures etc. can be used gainfully for weakly divergent quantities like specific heat etc.. The lattice models studied are the s.q. to s.c. and the s.q. to f.c.c. Ising models.

The plan of this dissertation is as follows. In Chap-

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The following results emerge from this study.

1. The detailed universal behaviour of the model near $g = 0$ is described by the extended scaling theory (4) quite accurately. We verify this by calculating the first five universal amplitude ratios.

2. The predictions of the theory about the double-power scaling laws, scale-factor universality etc. are verified and the universal parameters are calculated within an accuracy of 5%.

3. The universal scaling function for the dimensional cross-over for the susceptibility is obtained for all temperatures in the critical region. The graphs of the effective exponent are presented for a range of values of anisotropy in this regime. (5)

References :

1. L.J. de Jongh and A.R. Miedema, *Advances in Physics* 23, 1 (1974).
2. C. Domb in *Phase Transitions and Critical Phenomena*, Vol. 3, eds. C. Domb and M.S. Green (Academic, New York, 1974).
3. E.K. Riedel and F. Wegner, *Z. Physik* 225, 195 (1969).
4. P. Pfeuty, D. Jasnow and M.E. Fisher, *Phys. Rev.* B10, 2088 (1974).
- 5 (a) W.L. Basalawmoit and S. Singh, *Nucl. Phys. and Solid State Physics* 24C, 361 (1981).
(b) W.L. Basalawmoit and S. Singh, *Phys. Lett.* 88A, 251 (1982)
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Date : 10th January, 1983.

Surjit Singh

Signature of the Supervisor

Place : Shillong.

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Wendy Loslet Basaiawmoit
(Wendy Loslet Basaiawmoit)

Dated Shillong

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INTRODUCTION

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CONTENTS

Inner cover page.....	(i)
Supervisor's Certificate.....	(ii)
Acknowledgements.....	(iii)
Introduction.....	(iv)
CHAPTER 1 : : Introduction	
1.1. Brief History of Ising Model.....	1
1.2. Brief History of Scaling.....	4
and Universality	
1.3. Brief History of Crossover.....	13
Scaling and Universality	
1.4. Present Model.....	15
1.5. Summary of the Remaining.....	17
Chapters	
CHAPTER 2 : : Scaling Theory and Summary of Previous Work	
2.1. Scaling Theory and.....	18
its Predictions	
2.2. Summary of the Previous.....	22
work on the Present Model	
CHAPTER 3 : : Two-dimensional Behaviour	
3.1. Summary of the Extrapolation.....	25
Methods	
3.2. The Isotropic Behaviour.....	32
CHAPTER 4 : : Anisotropic Behaviour	
4.1. Introduction.....	49
4.2. Estimation of the Critical.....	50
Points and Critical Amplitudes	
4.3. Estimation of w and x	62

4.4.	Estimation of Critical Amplitudes A_{∞} and X	64
CHAPTER 5 : : Scaling Functions and the Effective Exponent		
5.1.	Introduction	68
5.2.	Scaling Function, Case (i)	71
5.3.	Scaling Function, Case (ii)	71
5.4.	The Effective Exponent	75
CHAPTER 6 : : General Remarks and Conclusion		
6.1.	General Remarks: Other Lattices and Related Models	83
6.2.	Comparison of our Results with others	84
6.3.	Concluding Remarks	86
References		88
Appendix :	List of Publications	95

TABLES

1.	Summary of definitions of..... 8 critical point exponents for magnetic systems. Here $t = \frac{T}{T_c} - 1$	8
2.	Rigorous results, for cross- 33 ing over from a quasi-2- -dimensional lattices to a true 3-dimensional lattice. The lattice coefficients are also defined	33
3a.	Reduced susceptibility ex-..... 35 pansion coefficients b_{n1} for the s,q to s.c. case	35
3b.	Same as 3a, but for the..... 38 s,q to f.c.c. case	38
4a.	Padé estimates for the iso-..... 41 tropic amplitudes for the s.c. lattice. The symbol '—' means a defective entry and n.c. means not calcula- ted. The estimates given here are related to the ac- tual estimates by the fol- lowing relations. $C_2 = 4K_c^2 C_2'$, $C_3 = 8K_c^3 C_3'$, $C_4 = 16K_c^4 C_4'$, $C_5 = 32K_c^5 C_5'$, $C_6 = 64K_c^6 C_6'$	41
4b.	Same as 4a, but for the 42 f.c.c. lattice. The rela- tions for this case are $C_2 = 112K_c^2 C_2'$, $C_3 = 2336K_c^3 C_3'$,	42

$$C_4 = K_c^4 C_4', \quad C_5 = K_c^5 C_5', \quad C_6 = K_c^6 C_6'$$

5a.	Pade estimates for the universal ratios for the s.c. lattice evaluated at $K=K_c(0)$. The symbol '—' means a defective entry, n.c. means not calculated	44
5b.	Same as 5a, but for the f.c.c. lattice	45
6.	Overall estimates for the universal amplitude ratios	46
7.	R_m Estimates of critical temperatures $K_c(g)$ for various values of g , for the s.c. and f.c.c. lattices. Extrapolation uncertainty is about 0.2%	56
8.	Estimates of the critical amplitudes $A(g)$ for various values of g , for the s.c. and f.c.c. lattices. Extrapolation uncertainty is about 4%	57
9.	Critical point shifts for the s.c. and f.c.c. lattices. Uncertainties in the last place are indicated in the brackets	59
10.	Estimates of the anisotropic amplitudes $A_{eff}(g)$ for the s.c. and f.c.c. lattices. Uncertainties in the last	63

place are indicated in the brackets

11. Coefficients of Padé approximants for various $P(z)$ for $\dot{x} = 1.334$ and $\dot{X} = 1.071$ 70
12. Same as 11, but for the case $\dot{x} = 1.530$ and $\dot{X} = 1.216$ 72
13. Values of non-universal parameters for various two- to three-dimensional cross-overs. 82

FIGURES

1.	Schematic isotherms of a.....5 typical ferromagnet	5
2.	Scaling functions for the.....6 magnetization both above and below T_c (schematic)	6
3.	Various special cases of.....11 the general n -vector ex- change model	11
4a.	Extrapolation of $\mu_n(g)$51 (see equation 4.2) ver- sus n^{-2} for various va- lues of g for the s.c. lattice. The parameter $\epsilon = -0.5$ for all of these	51
4b.	Same as 4a, but for the.....52 f.c.c. lattice	52
5a.	Extrapolation of $\bar{\mu}_n(g)$ 54 (see equation 4.3) ver- sus n^{-2} for various va- lues of g for the s.c. lattice	54
5b.	Same as 5a, but for the.....55 f.c.c. lattice	55
6a.	Plot of $w_{eff}(g)$ versus g60 for the s.c. lattice to obtain w	60
6b.	Same as 6a, but for the.....61 f.c.c. lattice	61
7a.	Extrapolation of $A_{eff}(g)$65 versus g , to get A_∞ for	65

	the s.c. lattice	
7b.	Same as 7a, but for the.....	66
	f.c.c. lattice	
8.	Plots of selected $P(z)$	73
	versus z for $0 \leq z \leq 1$.	
	The symbols (i), (ii)	
	and (iii) correspond to	
	the three choices men-	
	tioned in the text (see	
	equations 5.8, 5.9 and	
	5.10)	
9a.	Graphs of the effective.....	76
	exponent versus $\log t$	
	for the three choices	
	(i), (ii) and (iii) for	
	the f.c.c. lattice	
9b.	Same as 9a, but for the.....	77
	s.c. lattice	
10a.	The variations of the ef.....	78
	fective exponent as a	
	function of $\log t$ for	
	various values of g for	
	the f.c.c. lattice	
10b.	Same as 10a, but for the.....	79
	s.c. lattice	

INTRODUCTION

1.1. Brief History of Ising Model

Uhlenbeck and Goudsmit,¹ in 1925, put forward the hypothesis that the electron possesses a magnetic moment, and that, in a magnetic field its direction is quantized so that it orients itself either parallel or anti-parallel to the field. This extra degree of freedom is called spin. In the same year, Lenz suggested to his student Ising² that if an interaction was introduced between the spins so that parallel spins in a lattice attract one another, and anti-parallel spins repel one another, then at sufficiently low temperatures the spins would all be aligned and the model might provide a microscopic description of ferromagnetism. The corresponding Hamiltonian is of the form

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - mH \sum_i s_i, \quad (1.1)$$

Here $J (> 0)$ represents the interaction between spins, H is an external magnetic field, m the magnetic moment of a single spin and s_i is a dummy variable which can take the values ± 1 . The suffix i runs over all sites of the lattice and $\langle ij \rangle$ over all pairs of sites i and j which are nearest neighbours (n.n.). This is

called the Ising model. (For an interesting historical review of this model, see the article by Brush³).

Ising solved the model in one dimension and found that the solution is analytic without any singularities and the spontaneous magnetization vanishes for all $T > 0$. Eleven years later Peierls⁴ showed that the two-dimensional model does have a non-zero spontaneous magnetization and therefore can be regarded as a valid model of a ferromagnet. (For a summary of rigorous results on the Ising model, see the article by Griffiths in the Domb-Green Series⁵).

In 1941, Kramers and Wannier⁶ discovered a transformation which enabled them to calculate the exact value of the Curie temperature of a simple quadratic (s.q.) lattice. They also showed how to develop exact series expansions for the partition function at high and low temperatures. Their paper was followed by Onsager's famous calculation in 1944 of the partition function⁷ of the s.q. lattice in zero field, which has served as a landmark in the theory of critical behaviour. During subsequent years exact information was obtained on the Ising model as calculations were extended to the spontaneous magnetization,⁸⁻⁹ correlations¹⁰⁻¹¹ and susceptibility;¹¹⁻¹³ solutions also became available for a variety of additional two-dimensional lattices. (See the reviews by Domb¹⁴ and Syozi¹⁵). However, it has so far proved impossible to solve the model exactly in non-zero field or in three dimensions.

In the absence of exact solutions the two alternative approaches available were closed form approximations and series expansions. The former had been developed in the 1930s by Bragg and Williams,¹⁶ Bethe,¹⁷ Guggenheim¹⁸ and others. But, a comparison by Kramers and Wannier⁶ with exact series expansions showed that even the best approximations available gave only a

few terms correctly. Also such approximations were suggested by the authors to be unreliable in the critical region and this suggestion was substantiated by Onsager.⁷

Series expansions had been introduced by Kramers and Wannier⁶ with the aim of testing the validity of closed form approximations as mentioned above. However, Domb¹⁹ suggested that if expansions of sufficient length could be derived they might provide a direct assessment of critical behaviour. Such expansions were derived in two dimensions for the s.q. lattice by Domb¹⁹ and in three dimensions for the simple cubic (s.c.) lattice by Wakefield.²⁰ These calculations were extended to a variety of two- and three-dimensional lattices¹⁴ and methods of extracting information regarding critical behaviour were steadily improved.

Series for the initial susceptibility at high temperatures provided the smoothest and most regular pattern of behaviour of coefficients, they were all found to be positive in sign, and the ratio method²¹ was used to estimate the Curie temperatures and critical exponents. For the s.q. and plane triangular (p.t.) lattices in two dimensions, the Curie temperatures were known exactly, and hence a more accurate estimate could be made of the critical exponents. Domb and Sykes²² suggested the value $\gamma = 1.75$ for the susceptibility exponent of these lattices and this was later justified rigorously.^{11-13,23} For three-dimensional lattices the corresponding estimate²⁴ was 1.25.

A dramatic step forward was taken by Baker²⁵ in 1961 who applied Pade approximant²¹ to these Ising series. For series with positive terms, the results were in excellent accord with those of the ratio method. But for irregular series, e.g., the low temperature series for spontaneous magnetiza-

tion, it was possible to obtain estimates for the critical exponent of the spontaneous magnetization.

Due to the existence of the exact solutions and the possibility of deriving extensive series expansions both at low and high temperatures, the Ising model has served as a pioneer in the exploration of critical behaviour and many important results in the theory of critical phenomena started with application to the Ising model. These include accurate estimates of the critical exponents,^{24,26-28} accurate estimates of critical values of thermodynamic functions,¹⁴ observation that dimension rather than lattice structure determines critical behaviour of antiferromagnets,²⁹ critical amplitudes,^{30,31} critical equation of state,^{32,33} critical correlations,³⁴ surface and finite size effects,³⁵ lattice-lattice scaling,³⁶ correction terms to the equation of state,³⁷ the crossover exponent.³⁸

From all these and many more studies, it has now been established that, in general, the critical exponents depend on very few details of the system, e.g., the dimensionality, the symmetry properties of the Hamiltonian, etc. A systematic method of getting expansions for the exponents in terms of these parameters was introduced by Wilson and Fisher.³⁹ This so-called renormalization group method has been a valuable tool in getting numerical values for critical parameters, sometimes comparable in accuracy with the other methods. (Recent reviews are by Wilson and Kogut⁴⁰ and also by Fisher⁴¹).

1.2. Brief History of Scaling and Universality

The scaling hypothesis was introduced by Widom,⁴² Kadanoff,⁴³ Domb and Hunter,³² Patashinskii and Pokrovskii,⁴⁴

Fig. 1

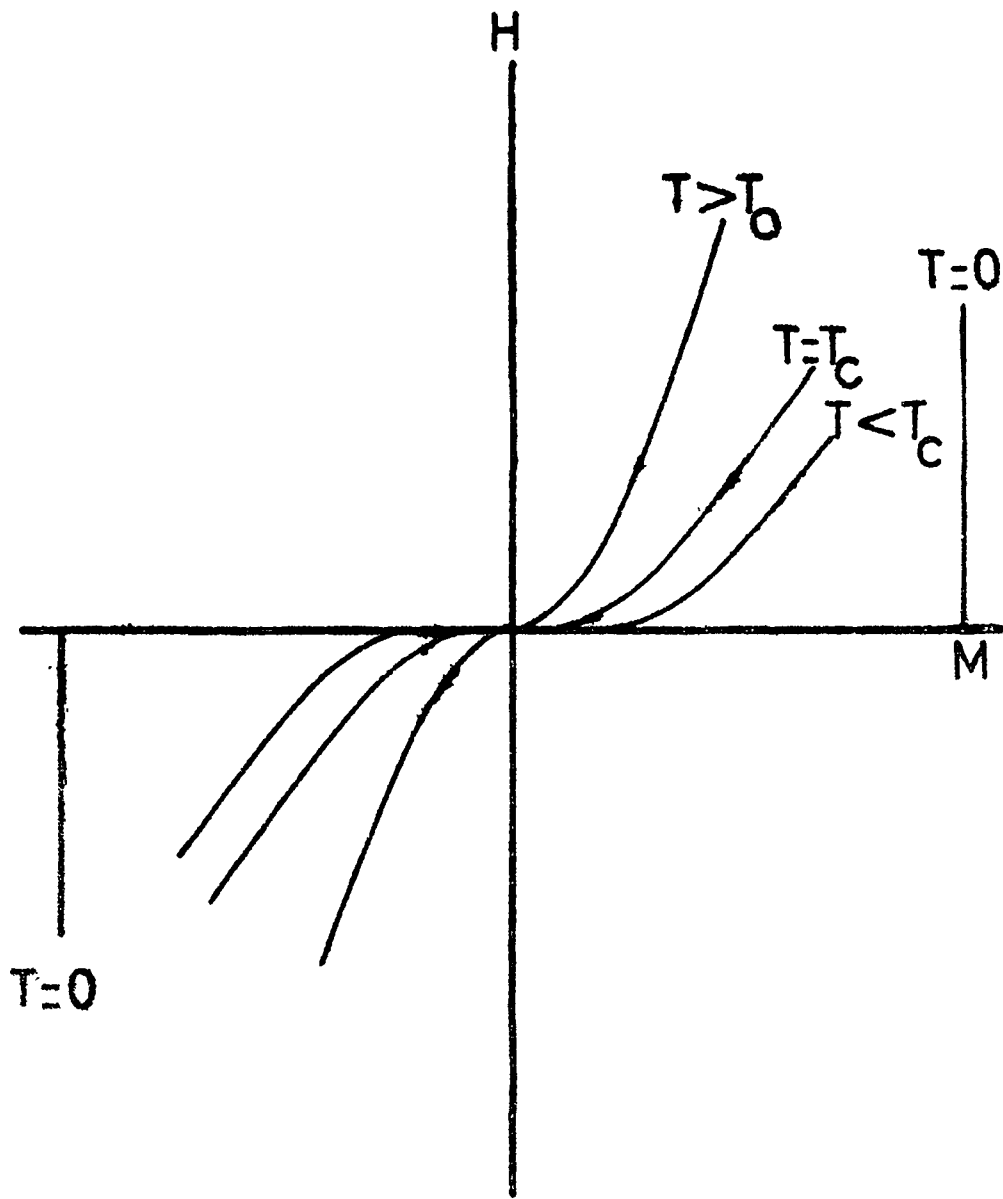
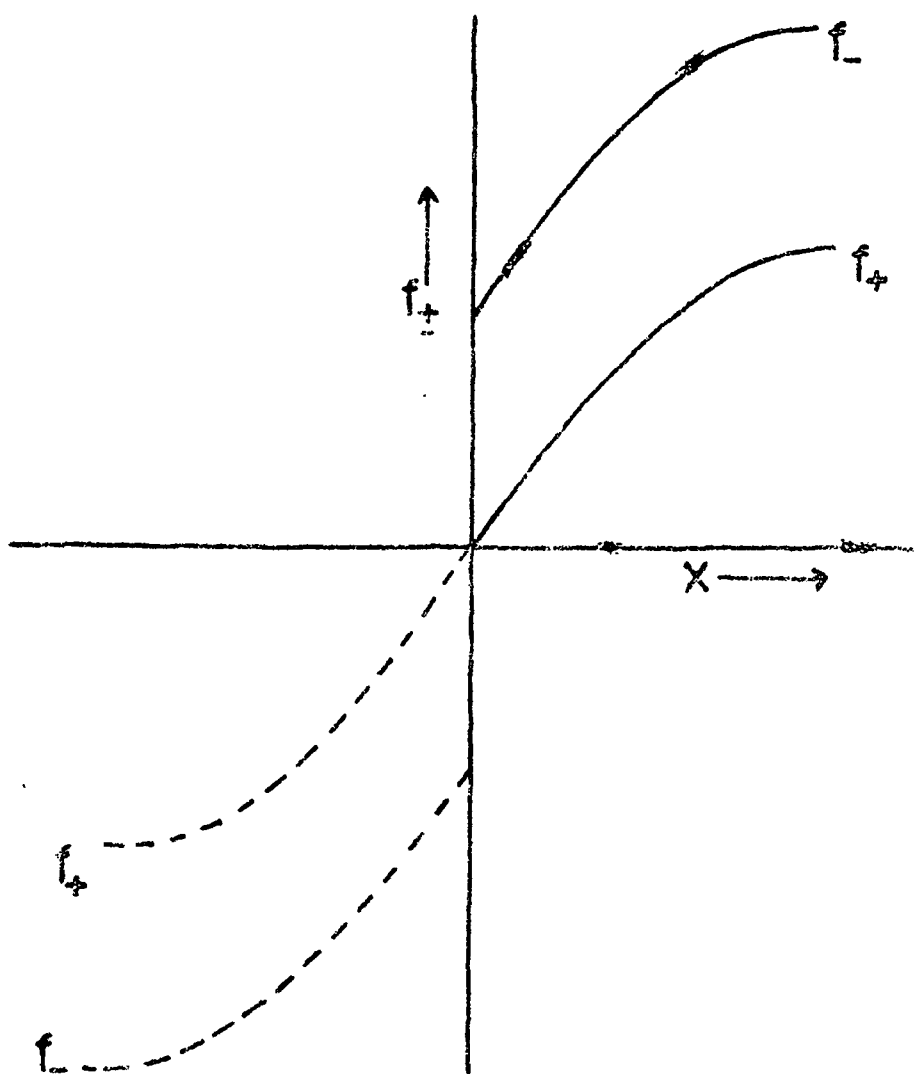


Fig. 2



more or less independently. (For recent reviews of these and other ideas see Fisher,⁴⁵ Stanley⁴⁶). The basic idea is to look at the isotherms in Figure 1 and notice that they are very similar to one another. The scaling hypothesis exploits this similarity to bring all the isotherms on one curve by introducing a change in scale which is temperature-dependent. The hypothesis states that

$$\frac{M(H,T)}{a|t|^\lambda} \approx f_{\pm} \left(\frac{bH}{|t|^\Delta} \right), \quad t = (T - T_c)/T_c, \quad (1.2)$$

where λ and Δ are two exponents and 'a' and 'b' are scale factors which have been introduced to make the scaling functions universal.^{47,48} The functions f_{\pm} are valid for $t > 0$ and $t < 0$, respectively. A typical sketch of functions f_{\pm} is shown in Figure 2. Following comments are to be noted regarding the hypothesis.

The symbol " \approx " denotes that it is valid in the critical region, i.e., for both H and t very small, typically $\lesssim 10^{-2}$. The variable $x = bH/|t|^\Delta$ has the range $-\infty \leq x \leq \infty$. The functions f_+ and f_- are different from each other owing to the fact that the isotherms for $T > T_c$ are essentially different from those for $T < T_c$. No particular value of x corresponds to the critical point ($H = 0, T = T_c$) because x is indeterminate for $H = 0, T = T_c$. However, there exists one value of x which corresponds to each path taken by an approach to the critical point. Of course, the hypothesis does what it was designed to do. If we change H and t by factors of l and $l^{1/\Delta}$ respectively, M is simply multiplied by $l^{-\lambda}$. In fact, this can be explicitly noted by writing (1.2) in the following form

$$M(H,t) \approx a l^{-\lambda} M(l^\Delta bH, lt), \quad (1.3)$$

Table 1. Summary of Definitions of Critical Point Exponents for Magnetic Systems. Here $t = \frac{T}{T_c} \sim 1$.

Exponent	Definition	Condition			Quantity
		t	H	M	
α'	$C_H \sim (-t)^{-\alpha'}$	0	0	0	Specific heat at constant magnetic field.
α	$C_H \sim t^{-\alpha}$	0	0	0	
β	$M \sim (-t)^\beta$	0	0	0	Zero-field magnetization.
γ'	$\chi_T \sim (-t)^{-\gamma'}$	0	0	$\neq 0$	Zero-field isothermal susceptibility.
γ	$\chi_T \sim t^{-\gamma}$	0	0	0	
δ	$H \sim M _{\text{sgn}(M)}^\delta$	0	$\neq 0$	$\neq 0$	Critical isotherm.

where l is arbitrary. In this form, it is called the generalized homogeneity hypothesis.⁴⁶

Now, we will study some of the implications of the scaling hypothesis.

β (a) For $H = 0$, we know that $\langle M \rangle = 0$ for $t > 0$ and $H = B|t|$ for $t \leq 0$. (For the sake of completeness, in Table 1, we give the standard definitions of the exponents^{45,46}). In order to reproduce this behaviour equation (1.2) should satisfy the following

$$f_{\pm}(0) = 0 \quad , \quad f_{-}(0) = 1 \quad , \\ \lambda = \beta \quad , \quad a = B .$$

(b) For $T = T_c$, $H \rightarrow 0^+$ a new exponent is defined for the shape of the critical isotherm.

$$M = D H^{1/\delta} \quad , \quad T = T_c \quad , \quad H \rightarrow 0 .$$

The functions $f_{\pm}(x)$ should satisfy the following conditions:

$$f_{\pm}(x) = x^{1/\delta} \quad , \quad x \rightarrow \infty \quad , \\ \lambda/\Delta = 1/\delta \quad , \quad D = a b^{1/\delta} .$$

(c) Differentiating equation (1.2) with respect to H , we get a scaling hypothesis for χ

$$\chi(H,t) \approx a b |t|^{\lambda-\Delta} f'_{\pm} \left(\frac{bH}{|t|^{\Delta}} \right) . \quad (1.4)$$

Using this, we can show that, e.g.,

$$\gamma = \gamma' = \Delta - \lambda .$$

Similarly, all other thermodynamic functions can be shown to obey the scaling hypothesis. So, all the thermodynamic exponents can be expressed in terms of just two exponents, viz., λ and Δ . By eliminating these one can get relations between exponents. Obviously, the number of independent rela-

tions will be two less than the number of exponents. An example of these relations²⁶ is

$$\gamma = \beta (\delta - 1) .$$

Similarly, all the amplitudes can be expressed in terms of just two amplitudes and the values of f_{\pm} and their derivatives at special points.^{47,48} The thermodynamic scaling has been verified experimentally in both fluids and magnets. The detailed predictions like the exponent relations have also been verified both theoretically and experimentally.^{49,50}

In order to understand the universality hypothesis, we should first note that all the quantities that characterize the critical behaviour of the system can be divided into two categories: Universal and Non-universal. Quantities which depend on very few properties of the system are called universal quantities, e.g., critical exponents and scaling functions. The remaining quantities which depend on details of the system are called non-universal quantities, e.g., critical temperature, critical amplitude and scale factors.

Most studies of universality^{41,50} have been devoted to the so-called "n-vector model" or the "general exchange Hamiltonian". The basic variables in the model are n-component classical unit vectors sitting on a d-dimensional lattice, interacting through a rotationally symmetric "exchange". The Hamiltonian is written as

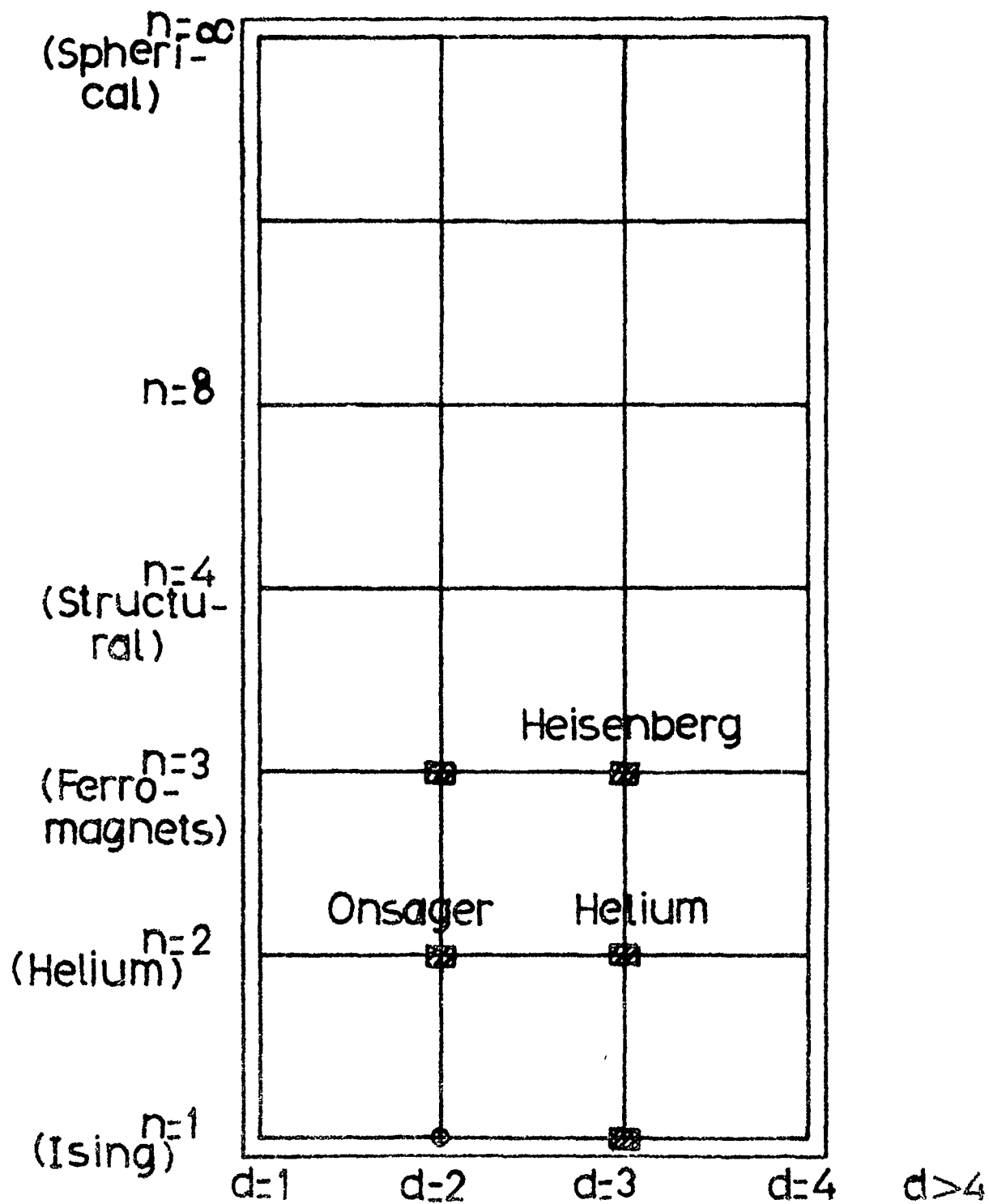
$$\mathcal{H} = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j \quad , \quad J > 0 \quad , \quad (1.5)$$

where $\vec{s}_i = \{s_i^\alpha, \alpha = 1, 2, 3, \dots, n\}$ satisfy the constraint

$$\sum_{\alpha=1}^n (s_i^\alpha)^2 = 1 .$$

The Hamiltonian has been studied in all its generalizations.^{41,50}

Fig. 3



Some examples are, differing exchanges in different lattice directions, in different spin directions; interactions becoming long ranged, etc.

Before discussing the results it is useful to point out that the Hamiltonian (1.5) provides a model for many interesting physical systems, as indicated in Figure 3. The values $n = 1, 2, 3$ are realized in magnetic materials. Superfluids are described by $n = 2$ and ordinary fluids, binary mixtures and alloys by $n = 1$. Recently, it has been shown that certain structural transitions can be described by $n = 4, 6, 8$.⁵¹ The limit $n \rightarrow \infty$ corresponds to the spherical model.⁵²⁻⁵⁴

The universal quantities depend on the following :

(i) Dimensionality d of the system, which is defined as the number of physical dimensions in which the system has infinite extent.

(ii) Symmetry number n , which is the number of independent components of the order parameter needed to describe the ordered state.

(iii) Range of interactions, short-range interactions are those satisfying $\sum_{R_i} R_i^2 J(R_i) < \infty$. All others are classified as long-range. When interactions are long-range, they are usually taken to be $J(R) \sim R^{-(d+\sigma)}$ for $R \rightarrow \infty$. For $0 < \sigma < 2$, the interactions are long-range and the exponents are σ -dependent in general.⁴¹

The universal quantities do not depend on the details of lattice structure, the length of the system in the direction in which it is finite, and the strength of the interactions in different directions. They are also independent of the magnitude of the spin quantum number $S = \frac{1}{2}, 1, \frac{3}{2}, \dots, \infty$, number of spin components, amount of anisotropy in the spin space as long as it does not change the symmetry properties of the Hamiltonian.

Lastly, they do not depend on the strength of the next nearest (or more) neighbours as compared with that of nearest neighbour interactions.

The basic reason for universality is the existence of long-range correlations near the critical point. Due to their range, they do not "see" the details of the system, but only the gross features like the dimensionality, symmetry properties, etc.

Summing up, to each set of (d, n, σ) corresponds a unique set of two independent thermodynamic exponents and a unique scaling function. Systems having the same (d, n, σ) are said to belong to the same universality class. A natural question is as to how one extrapolates between different universality classes. This leads naturally to crossover phenomena which is the subject of the next section.

1.3. Brief History of Crossover Scaling and Universality

Crossover occurs when the exponents of the system change discontinuously at a special point when a parameter, say g , is changed continuously. Let us call the special value of g zero. Then, for $g = 0$, we have one set of exponents α , β , γ , etc. And, by the universality hypothesis, for $g \neq 0$, we have another set of exponents, say, α' , β' , γ' , etc. For convenience, let us call the $g = 0$ and $g \neq 0$ systems as the isotropic and anisotropic systems, respectively.

According to the crossover scaling theory,^{55,56} which is developed systematically in Section 2.1, one expects that for weak anisotropy, the system behaves first as if fully iso-

tropic when the critical point is approached. However, on going closer to the critical temperature $T_c(g)$, the system starts to respond to the anisotropy until, eventually, its behaviour becomes fully characteristic of $g \neq 0$ systems. The change to anisotropic form occurs in the vicinity of a crossover temperature $T^x = T_c(g) + \Delta T^x$ whose variation is determined by a crossover exponent ϕ according to $\Delta T^x \sim g^{1/\phi}$. The value of ϕ is characteristic of the isotropic system and the type of crossover involved but, as usual, should not depend on the details of lattice structure, etc.

To describe this behaviour, a scaling hypothesis for the case of spin-space anisotropy (e.g., Heisenberg to Ising crossover) in terms of the variables g/t^ϕ , where

$$t = [T - T_c(g)] / T_c(0) \quad , \quad (1.6)$$

was made by Riedel and Wegner.⁵⁵ They verified the predictions of the theory in the mean-field approximation and in the spherical model. This, however, left open the value of the shift exponent Ψ , defined as

$$T_c(g) - T_c(0) \approx g^{1/\Psi} \quad , \quad g \rightarrow 0 \quad .$$

This question was discussed in detail by Fisher and Jasnow⁵⁶ (unpublished). They showed that, in general, Ψ may or may not be equal to ϕ . If $\Psi = \phi$, then one can make an extended scaling hypothesis in terms of the variables g/t^ϕ where

$$t = [T - T_c(0)] / T_c(0) \quad . \quad (1.7)$$

Conversely, if the extended form is assumed, then the conclusion $\Psi = \phi$ is forced. If $\Psi \neq \phi$, then the extended scaling can still be made but in terms of more complicated variables. (For many examples of this last case, see Singh⁵⁷ (unpublished)).

To see the kind of crossovers that are possible in physical systems, let us turn to Figure 3. Let us denote each point by its co-ordinates (d,n) . (We restrict ourselves to the case of short-range forces, for simplicity). In principle, each point is characterized by a different set of exponents, so we can have crossover from any one point to another. Most thoroughly studied, theoretically as well as experimentally, are the cases $(3,3)$ to $(3,2)$ and $(3,1)$. All the predictions were verified and scaling functions were obtained theoretically by Pfeuty, Jasnow, Fisher and Singh.⁵⁸⁻⁶⁰ These results had a direct application in Heisenberg systems exhibiting a bicritical point.⁶¹ Such points were studied experimentally by Rohrer⁶² who found good agreement between theory and experiment. Various crossovers in the spherical model were studied by Riedel and Wegner⁵⁵ and Singh and Jasnow⁶³ (unpublished). The only other case which has been studied in some detail is the $(2,1)$ to $(3,1)$ case by Stanley and coworkers.⁵⁰ We discuss their work in Section 2.2 in detail. Many other interesting crossovers have been studied mainly by the renormalization group techniques. (For a recent review see the article by Aharony⁶⁴). In the coming section we introduce the present model.

1.4. Present Model

Onsager's paper⁷ on the two-dimensional Ising model also contained a discussion of the anisotropic rectangular lattices with different interactions J and J' in the two principal lattice directions. This work has been extended to the spontaneous magnetization in the anisotropic lattice (see Domb¹⁴). For these exact solutions, critical exponents remain unchanged as long as $J' \neq 0$.

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The smoothness postulate⁶⁵ generalizes this result to any isotropic system in d dimensions. For example, if we consider a set of parallel s.q. lattices with **intra** interactions J coupled to one another with interaction J' , we should expect the system to display three-dimensional critical exponents as long as $J' > 0$, and to revert to two-dimensional exponents only when $J' = 0$.

In this work, we shall be dealing with quasi-two-dimensional systems, i.e., three-dimensional systems in which the interactions in the off-plane directions are weaker than those within the planes. The most important parameter determining the behaviour of such a system is the lattice-anisotropy, g , i.e., the ratio of the interplanar to intraplanar couplings. For g large, say more than 10^{-2} or so, the properties of the system are essentially three-dimensional in nature. So one can use the standard Padé approximant method to construct the thermodynamic functions for all temperatures.⁶⁶ On the other hand, for smaller values of g , the crossover behaviour makes itself felt, so more refined techniques must be used.

Our model is the ferro-magnetic quasi-two-dimensional Ising model without magnetic field. The interactions which are purely in the xy -plane are denoted by J and all others by J' . The anisotropy parameter is $g = J'/J = J_z/J_{xy}$. The two lattices studied are the s.c. and face-centered cubic (f.c.c.) lattices. We are considering a crossover from 2-d to 3-d. The Hamiltonian of our model is

$$H = -J \sum_{\langle ij \rangle}^{xy} s_i s_j - gJ \sum_{\langle ij \rangle}^z s_i s_j, \quad s_i = \pm 1, \quad J > 0. \quad (1.8)$$

The first summation runs over all the n.n. pairs of spins in the xy -plane, and the second summation is over all other n.n. pairs. For $g = 0$, the Hamiltonian describes a set of mutually non-interacting two-dimensional Ising models. For $g = 1$, it

describes either the s.c. or f.c.c. model.

In Chapters 3 to 5, we will study the crossover scaling behaviour of this model in detail. Such models have also been studied experimentally. (For a recent review, see de Jongh and Miedema⁶⁷). The only known example of the present model is perhaps FeCl_2 . But in this case, the value of g is estimated to be 8×10^{-2} , so it is outside the crossover scaling region. Further experimental studies on such systems would be most welcome.

The coming section gives the summary of all the remaining chapters.

1.5. Summary of Remaining Chapters

The outline of the remaining chapters is as follows. In Chapter 2, the crossover scaling theory is presented. Also given is a summary of previous work on the same model. In Chapter 3, the low- g expansion of the scaling function is obtained through the analysis of the isotropic critical behaviour of the susceptibility. The study of the critical behaviour in the presence of small but finite anisotropy is the subject of Chapter 4. In Chapter 5, we construct the closed form approximants for the scaling function and we also examine the crossover of the susceptibility exponent based on this function. Chapter 6 which is the last chapter contains a summary of the work done and also our concluding remarks.



Scaling Theory and Summary of Previous Work

2.1. Scaling Theory and its Predictions.

In this Chapter, we shall obtain the detailed predictions of the scaling theory as applied to the ferromagnetic quasi-two-dimensional Ising model Hamiltonian (1.8),

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - gJ \sum_{\langle ij \rangle} s_i s_j, \quad s_i = \pm 1, \quad J > 0. \quad (1.8)$$

For $g = 0$, the Hamiltonian (1.8) describes a set of mutually non-interacting two-dimensional Ising models. The zero-field reduced susceptibility is given by,

$$\chi(g=0, T) \approx A t^{-\gamma}, \quad (2.1)$$

where,

$$t = [T - T_c(0)] / T_c(0), \quad (2.2)$$

in the critical region. So, in the absence of anisotropy, the critical behaviour is described by the usual critical exponents $\alpha, \beta, \gamma, \dots$. But if anisotropy is present, the critical temperature is shifted from $T_c(0)$ to $T_c(g)$ and the critical

behaviour is described by the new exponents $\dot{\alpha}$, $\dot{\beta}$, $\dot{\gamma}$
Thus for $g \neq 0$, it is convenient to introduce

$$\dot{t} = [\tau - \tau_c(g)] / \tau_c(0) \quad (2.3)$$

The susceptibility is then given by,

$$\chi(q, \tau) \approx \dot{A}(g) \dot{t}^{-\dot{\gamma}}, \quad \dot{t} \rightarrow 0 \quad (2.4)$$

For small \dot{t} and small g , the general scaling theory⁵⁵ implies that the zero-field susceptibility should be of the form,

$$\chi(q, \tau) \approx A \dot{t}^{-\dot{\gamma}} X_1(B_1 g / \dot{t}^\phi), \quad (2.5)$$

where ϕ is the crossover exponent and the scale factors A, B , have been introduced to make the scaling function $X_1(x)$ universal. Now for $g = 0$, we should get (2.1). Therefore, we must have

$$X_1(x) \rightarrow 1, \quad x \rightarrow 0.$$

On the other hand, to reproduce (2.4), $X_1(x)$ must go to zero as $x \rightarrow \infty$ as follows,

$$X_1(x) \approx X_1 x^{(\dot{\gamma} - \gamma)/\phi}, \quad x \rightarrow \infty$$

Substituting this in (2.5), we get

$$\chi(q, \tau) \approx A \dot{X}_1(B_1 g) \dot{t}^{-(\dot{\gamma} - \gamma)/\phi - \dot{\gamma}},$$

so that,

$$\dot{A}(g) \approx A \dot{X}_1(B_1 g)^{(\dot{\gamma} - \gamma)/\phi}.$$

This is the so-called double power law scaling prediction.

The hypothesis (2.5) leaves open the question of the variation of the critical point shift,

$$t_c(g) = [T_c(g) - T_c(0)] / T_c(0) , \quad (2.6)$$

with g , for small g . One may, indeed,^{56,58} introduce a new shift exponent Ψ through

$$t_c(g) \sim g^{1/\Psi}$$

As mentioned before in Section 1.3, it can be shown that if $\Psi = \phi$, then the extended scaling theory applies and vice versa. The extended scaling theory implies that

$$\chi(g, T) \approx A t^{-\gamma} X(Bg/t^\phi) . \quad (2.7)$$

We shall exclusively work with this extended form of the theory, which means, e.g., that we put $\Psi = \phi$. (Of course, the two scaling functions $X(x)$ and $X_1(x)$ are simply related).

Now, we summarize the detailed predictions of the theory following Pfeuty, Jasnow and Fisher.⁵³ Henceforth, this paper will be referred to as PJF. The successive derivatives of the zero-field susceptibility at $g = 0$ should diverge as

$$\Xi_m \equiv \left(\frac{\partial^m \chi}{\partial g^m} \right)_0 \approx C_m t^{-(\gamma + m\phi)} , \quad t \rightarrow 0 . \quad (2.8)$$

The scaling function $X(x)$ may be normalized by

$$X(0) = 1 , \quad \left(\frac{dX}{dx} \right)_0 = 1 . \quad (2.9)$$

Thus, we can easily see that,

$$C_0 = A , \quad C_1 = AB ,$$

and

$$C_m = AB^m \left(\frac{d^m X}{dx^m} \right)_0 . \quad (2.10)$$

Since the scaling function $X(x)$ is universal, the ratios of the amplitudes,

$$R_m = \frac{C_{m-1} C_{m+1}}{C_m^2}, \quad m = 1, 2, 3, \dots$$

are predicted to be universal.

For fixed positive g , however, we require equation (2.4) to be satisfied as $t \rightarrow 0$, i.e., $T \rightarrow T_c(g)$. To reproduce this behaviour, the susceptibility in the extended form (2.7) must be singular at $t = t_c(g)$ which, in accord with the equality $\phi = \Psi$, can be written as

$$t_c(g) = \dot{\omega} g^{1/\phi}, \quad \text{as } g \rightarrow 0 \quad (2.11)$$

The scaling function $X(x)$ itself, for $g \neq 0$, should be singular at x , say, to reflect the crossover to the new exponent $\dot{\gamma}$. The extended theory makes the simplest assumption, viz.,

$$X(x) \approx \dot{X} \left(1 - \frac{x}{\dot{x}}\right)^{-\dot{\gamma}}, \quad x \rightarrow \dot{x}. \quad (2.12)$$

This results in the following predictions. The quantity x is universal and is given by

$$\dot{x} = B \dot{\omega}^{-\phi}. \quad (2.13)$$

The amplitudes $\dot{A}(g)$ in (2.4) diverge as

$$\dot{A}(g) = A_\infty g^{(\dot{\gamma} - \gamma)/\phi}, \quad g \rightarrow 0,$$

with

$$\begin{aligned} A_\infty &= A \dot{X} \dot{\omega}^{\dot{\gamma} - \gamma} \phi^{-\dot{\gamma}} \\ &= A B^{(\dot{\gamma} - \gamma)/\phi} \dot{X} x^{(\gamma - \dot{\gamma})/\phi} \phi^{-\dot{\gamma}}. \end{aligned} \quad (2.14)$$

The universal amplitude \dot{X} can be obtained from (2.14),

$$\dot{X} = A_{\infty} \phi^{\dot{\gamma}} \dot{w}^{\gamma - \dot{\gamma}} / A \quad (2.15)$$

The parameters \dot{x} and \dot{X} are universal, while A, B, \dot{w} and A_{∞} are non-universal.

After this brief summary of the scaling theory, we summarize previous work in the coming section.

2.2. Summary of the Previous Work on the Present Model

We start with a summary of two-dimensional Ising models to which the present model reduces for $g = 0$. A beginning was made by Kramers and Wannier⁶ who showed that the model possesses a symmetry property, which permits location of the Curie temperature if it exists and is unique. It was found that it lies at

$$\begin{aligned} K_c(0) = J / k_B T_c(0) &= \frac{1}{2} \ln(1 + \sqrt{2}) \\ &= 0.440686793\dots, \end{aligned} \quad (2.16)$$

The symmetry also excludes certain forms of singularities at T_c , e.g., a jump in the specific heat. Onsager,⁷ in his paper on a two-dimensional model with an order-disorder transition computed, rigorously, the partition function of the two-dimensional s.q. model for the case of vanishing field. He showed that the specific heat is logarithmically singular at T_c given by Kramers and Wannier. His calculation showed for the first time that the formulation of statistical mechanics is capable of describing phase transitions and critical phenomena without any extra assumptions. An initial study of the susceptibility for the s.q.

lattice was done by Domb and Sykes²² who suggested that $\gamma = \frac{7}{4}$. A theoretical justification for this value was first given by Fisher¹² and the argument has subsequently been made completely rigorous.⁶⁸

Now we summarize the work on the quasi-two-dimensional models. The method of series expansions for $\chi(g, T)$ for the above model of the anisotropic s.c. lattice was used by Oitmaa and Enting.^{69, 70} Writing

$$\chi(g, T) = 1 + 2 \sum_{l=1}^{\infty} H_l(g) w^l, \quad w = \tanh k, \quad (2.17)$$

they evaluated the first eleven polynomials $H_l(g)$. By performing ratio and Pade approximant (P.A.) analysis for different g values, they found a continuous variation of the critical exponent γ with g which, they claimed, conflicted with the smoothness postulate predictions of a sharp change at $g = 0$. Rapaport⁷¹ pointed out that such a continuous variation must be expected from a finite number of terms in (2.17). This is due to the fact that as g approaches zero, more and more terms are required to indicate the true behaviour of the critical exponent. Using an alternative analysis which attempted to estimate the critical exponents of the isotropic derivatives of $\chi(g, T)$, i.e., Ξ_m (see equation 2.8), Rapaport showed that the data were consistent with $\phi = 1.75 = \gamma$. Therefore, he concluded that the data did not conflict with universality and smoothness. Similar conclusions were drawn by Paul and Stanley,⁷² who had independently developed high-temperature series expansions for the anisotropic s.c. and f.c.c. lattices. Rapaport's conclusions were again challenged by Enting and Oitmaa⁷³ who estimated the value of the exponent ϕ which was different from 1.75 and suggested that the scaling theory was not obeyed.

Liu and Stanley,⁷⁴ Cittert and Kasteleyn⁷⁵ resolved

the controversy by proving rigorously that $\phi = \gamma$. Also Harbus and Stanley⁷⁶ developed general-g series for the specific heat, susceptibility and second correlation moment for the anisotropic s.c. and f.c.c. lattices and these series were subsequently analysed by Krasnow et al.⁷⁷ who found good evidence in support of scaling.

This problem has been attacked by renormalization group approach. Using this method, Grover⁷⁸ and Chang and Stanley⁷⁹ showed that $\phi = \gamma$ for the general case of lattice dimensionality crossover. Also, Bruce⁸⁰ studied the problem of obtaining crossover scaling functions for this case.

In the next chapter, we give a brief summary of the extrapolation methods and obtain the $g = 0$ scaling behaviour. The $g \neq 0$ behaviour is discussed in Chapter 4.

Two-dimensional Behaviour

3.1. Summary of the Extrapolation Methods

Before studying the model for $g = 0$ and $g \neq 0$, in this section, we give a brief summary of the extrapolation methods for analysing the power series expansions.²¹ They are the ratio method and ~~Padé approximant~~ (P.A.) methods.

Ratio method is generally used to determine the location and nature of a dominant singularity which lies on the real axis. Let us assume that the dominant singularity of some function $F(K)$ is on the real axis at $K = K_c$, and that all the coefficients in the series are real and of one sign. Suppose that the function $F(K)$ has a power series of the form

$$F(K) = \sum_{n=0}^{\infty} a_n k^n \quad (3.1)$$

about the origin $K = 0$. If

$$\lim_{n \rightarrow \infty} |a_n|^{-1/n} = K_c, \quad (3.2)$$

then the series converges for $|K| < K_c$ and diverges for $|K| > K_c$. Correspondingly, there must be at least one singularity (non-analytic point) on the circle of convergence $|K| = K_c$. It follows from (3.2) that

$$a_n \approx f(n) K_c^{-n}, \quad K \rightarrow K_c, \quad (3.3)$$

or, more precisely,

$$\lim_{n \rightarrow \infty} [a_n K_c^n / f(n)] = 1. \quad (3.4)$$

where the unknown function, $f(n)$, satisfies

$$\lim_{n \rightarrow \infty} [f(n)]^{1/n} = 1. \quad (3.5)$$

For $f(n)$ let us consider the form

$$f(n) = A \binom{\gamma + n - 1}{n} = A \frac{\gamma(\gamma+1)(\gamma+2)\dots(\gamma+n-1)}{n!} \quad (3.6)$$

which behaves asymptotically like

$$f(n) \approx \frac{A n^{\gamma-1}}{\Gamma(\gamma)}, \quad (3.7)$$

where $\Gamma(\gamma)$ is the gamma function. The form for $f(n)$ implies that for $\gamma > 0$ and real K , we have,

$$F(K) = A \left(1 - \frac{K}{K_c}\right)^{-\gamma} \left[1 + O\left(1 - \frac{K}{K_c}\right)\right], \quad K \rightarrow K_c. \quad (3.8)$$

Evidently, the parameters γ and A directly determine the critical exponent and amplitude respectively, at the singularity. If we assume that the various singularities are power laws, equation (3.8) justifies (3.6) and (3.7) as the natural choice for $f(n)$.²² Following Domb and Sykes,²² consider the ratio of successive coefficients,

$$p_n = \frac{a_n}{a_{n-1}}, \quad n = 1, 2, 3 \dots \quad (3.9)$$

From (3.3) and (3.8), we expect

$$p_n = K_c^{-1} \left[1 + \frac{\gamma-1}{n} + O\left(\frac{1}{n^2}\right) \right], \quad n \rightarrow \infty \quad (3.10)$$

so that the ratios vary linearly with $\frac{1}{n}$ as $n \rightarrow \infty$. The intercept on $\frac{1}{n} = 0$ will give K_c and the slope gives $(\gamma - 1)/K_c$, from which γ can be determined. But if only a limited number of terms are known, we can only hope that the initial ratios will be sufficiently well-behaved as to enable an accurate extrapolation to be made. This depends, amongst other things, on the proximity and nature of any other singularities.

Knowing the estimated values of the critical point and critical exponent by the above method, we can also have refined estimates of each of them having known one of them first. Thus, given the exact value of the critical point K_c , or an estimated value K_c' , one may form the sequence of approximations²²

$$\gamma_n = n (p_n K_c' - 1) + 1 \quad (3.11)$$

According to (3.10)

$$\gamma_n \approx \gamma \left[1 + O\left(\frac{1}{n}\right) \right] + 1, \quad n \rightarrow \infty \quad (3.12)$$

so that γ_n should approach γ linearly against $\frac{1}{n}$, provided K_c' is sufficiently accurate. A modified version of (3.11), namely,

$$\gamma_n(\epsilon) = (n+\epsilon) (p_n K_c' - 1) + 1, \quad (3.13)$$

is sometimes used, where ϵ is a small shift which generally helps to improve convergence.

If one has the exact value of critical exponent γ , or a good estimate γ' , one can usually obtain a rapidly convergent sequence of estimates for the critical point K_c from the sequence²⁴

$$\left(K_c^{*-1}\right)_n \equiv \frac{n f_n}{n + \gamma - 1} \approx K_c^{-1} \left[1 + O\left(\frac{1}{n^2}\right)\right], n \rightarrow \infty. (3.14)$$

Since the leading correction term is of the order $O\left(\frac{1}{n^2}\right)$, the limit K_c^{-1} should be approached horizontally versus $\frac{1}{n}$. Even if γ' is somewhat different from γ , this will affect the convergence only through a term $(\gamma - \gamma')/n$.

If the critical point K_c and critical exponent γ are known accurately, the amplitude of singularity may be estimated (equations 3.3 and 3.6) from the sequence⁸¹

$$A_n = \frac{a_n K_c^n}{\binom{\gamma + n - 1}{n}} \quad (3.15)$$

Equations (3.3) and (3.6) suggest the alternative sequence

$$A_n = a_n K_c^n \frac{\Gamma(\gamma)}{n^{\gamma-1}} \quad (3.16)$$

but this is not usually very satisfactory. However, small errors in K_c and γ are magnified in estimating the amplitude A , so that comparatively lower accuracy is obtained.

The main failure of the ratio method is that in most cases it deals with only one singularity at a time and also if this singularity lies on the real axis and is dominant. If the ratios of the successive coefficients are oscillating wildly

in sign as well as magnitude, which implies that the singularity closest to the origin is in the complex plane and is not the physical singularity, then the ratio method fails completely. In such a case, P.A. method can be used successfully.

Pade' approximants enable several singularities lying anywhere in the complex K -plane to be studied simultaneously, in a systematic manner. In effect, they provide a method of approximately analytically continuing a function beyond its radius of convergence and up to the physical singularity, or beyond. Pade' method can also be applied to a series of all positive coefficients. It was introduced into physics by Baker and Gammel⁸² and Baker et al.,⁸³ and first applied to critical phenomena by Baker.²⁵

The $[L, M]$ P.A. to a function $F(K)$ is the ratio of a polynomial $P_L(K)$ of degree L to a polynomial $Q_M(K)$ of degree M . Thus we have,

$$[L, M] \equiv \frac{P_L(K)}{Q_M(K)} \equiv \frac{p_0 + p_1 K + p_2 K^2 + \dots + p_L K^L}{q_0 + q_1 K + q_2 K^2 + \dots + q_M K^M} \quad (3.17)$$

Without any loss of generality, we can assume $q_0 = 1$. The coefficients $p_0, p_1, p_2, \dots, p_L$ and q_1, q_2, \dots, q_M are chosen that the expansion of $[L, M]$ agree with the expansion of $F(K)$ through order $L + M$, i.e.,

$$F(K) = [L, M] + O(K^{L+M+1}) \quad (3.18)$$

Equating the coefficients of K^{L+1} through K^{L+M} in (3.17) gives M simultaneous linear equations for q_1 to q_M . Substituting their solution into the $(L+1)$ linear equations, obtained by equating the coefficients of K^0 through K^L in (3.18), then yields the coefficients p_0 to p_L .

If the series expansion of $F(K)$ is known through order K^N , the calculable approximants can be arranged in a Padé table⁸⁴ as follows

$$\begin{array}{ccccccc}
 [1,1] & [2,1] & \cdot & \cdot & \cdot & \cdot & [N-1,1] \\
 [1,2] & [2,2] & \cdot & \cdot & \cdot & \cdot & [N-1,2] \\
 \cdot & & & & & & \\
 \cdot & & & & & & \\
 \cdot & & & & & & \\
 \cdot & & & & & & \\
 [1,N-1] & & & & & &
 \end{array}$$

Applying this method to the series for a function $F(K)$ given in (3.1) we find that if $A(K)$ is analytic at $K = K_c$, then:

$$F(K) \approx A \left(1 - \frac{K}{K_c}\right)^{-\gamma} \left[1 + O\left(1 - \frac{K}{K_c}\right)\right], \quad (3.19)$$

where $A = A(K_c)$. It follows that the logarithmic derivative

$$D(K) \equiv \frac{d}{dK} \ln F(K) \approx \frac{-\gamma}{(K - K_c)} \left[1 + O(K - K_c)\right]_{K \rightarrow K_c} \quad (3.20)$$

has a simple pole at K_c .⁸² Since P.A. can represent simple poles exactly, approximants to the $D(K)$ series should converge much faster than approximants to the $F(K)$ series. If an approximant has a pole in the vicinity of K_c , its location will give the estimate of K_c while the corresponding residue will be an estimate of $-\gamma$.

If the exact value of a good estimate of γ is given, then the appropriate poles of the approximants to the series for

$$\left[F(K)\right]^{1/\gamma} \approx -\frac{K_c A^{1/\gamma}}{(K - K_c)} \left[1 + O(K - K_c)\right], \quad K \rightarrow K_c, \quad (3.21)$$

should give a more rapidly convergent sequence of the estimates for K_c .²² The corresponding residues yield estimates of $-K_c A^{1/\gamma}$, and hence the amplitude A .

Conversely, if the exact value or a good estimate of K_c is known, a better estimate of the critical exponent can be obtained by forming P.A._n to the series

$$\gamma^*(K) \equiv (K_c - K) D(K) \approx \gamma + O(K - K_c), \quad K \rightarrow K_c \quad (3.22)$$

and evaluating them at $K = K_c$.

If both K_c and γ are known accurately enough, better estimates of A can be obtained²⁶ by forming P.A._n to the series for

$$(K_c - K) [F(K)]^{1/\gamma} \approx K_c A^{1/\gamma} + O(K - K_c), \quad K \rightarrow K_c \quad (3.23)$$

evaluating them at K_c and raising the result to the power γ . In addition, one of the higher order approximants should provide an excellent extrapolation for $F(K)$ over the entire range from $K = 0$ to K_c .²⁶

In summary, Pade' method can be expected to work reasonably well whenever $F(K)$ diverges strongly to infinity or converges strongly to zero at K_c . This is the case for the high-temperature susceptibility series and low-temperature spontaneous magnetization series, respectively, of the ferromagnetic Ising model. If $F(K)$ has singularities at several points in the complex K -plane, the Pade method attempts to treat each of them. For example, if enough series coefficients are available, the location and exponent of singularity may be approximated by an appropriate pole and residue of the higher-order approximants to $D(K)$.

In addition to these general methods, there are special methods to analyse the crossover behaviour of the scaling function. We discuss and apply them in the coming sections.

3.2. The Isotropic Behaviour

In this section, we will deal with the $g = 0$ or, isotropic, behaviour of the Hamiltonian (1.8). We will deal with the cases s.q. to s.c. and s.q. to f.c.c. For $g = 0$, we get a set of s.q. Ising models. For the s.q. model, the critical temperature is given by (2.16) and the critical exponent γ is equal to $7/4$. The amplitudes A for $\chi(0, T)$ was obtained by Sykes and coworkers³¹ who analysed the high-temperature series for the two-dimensional Ising model. They found that near T_c the ferromagnetic susceptibility behaves as

$$\chi(0, T) \approx A \left(1 - \frac{T_c}{T}\right)^{-7/4} + A' \left(1 - \frac{T_c}{T}\right)^{-3/4}, \quad T \rightarrow T_c^+ \quad (3.24)$$

with $A = 0.96259 \pm 0.00003$, $A' \approx 0.0742$. These values are in excellent agreement with the exact values obtained by Barouch, McCoy and Wu.²³ They obtained

$$A = 0.9625817322 \dots, \quad A' = 0.0749381538 \dots \quad (3.25)$$

(We remark in passing about the confluent singularities in the asymptotic behaviour of the susceptibility in equation (3.24). We have not included these in our analysis, since we feel that the series are probably too short to examine all the subtle effects taking place for small values of g . We have concentrated only on the leading crossover behaviour for small g).

Knowing the value of A , the value of B can be obtain-

Table 2. Rigorous Results, for Crossing Over from a Quasi-2-dimensional Lattices to a true 3-dimensional Lattice. The Lattice Coefficients are defined below. Here

Physical Quantity	Lower Bound	Upper Bound	Range of (T,H)
$\left[\frac{\partial}{\partial g} C_H(T,H,g) \right]_{g=0}$	$-\frac{1}{2} N g_1 J T \frac{\partial^2}{\partial T^2} [M^2]$		Arbitrary.
$\left[\frac{\partial}{\partial g} \bar{\chi}(T,H,g) \right]_{g=0}$	$g_1 K M_0 \frac{\partial}{\partial h} \bar{\chi} + g_1 K \bar{\chi}^2$		Arbitrary.
$\left[\frac{\partial^2}{\partial g^2} \bar{\chi}(T,H=0,g) \right]_{g=0}$	$2g_{21} K^2 \bar{\chi}^3$	$2(g_{21} + g_{22}) \times K^2 \bar{\chi}^3$	$T > T_c, H=0.$
$\left[\frac{\partial^3}{\partial g^3} \bar{\chi}(T,H=0,g) \right]_{g=0}$	$(6g_{31} - 2g_{33}) \times K^3 \bar{\chi}^4$	$(6g_{31} + 12g_{32} + 6g_{33}) K^3 \bar{\chi}^4$	$T > T_c, H=0.$

Lattice Coefficients.

g	s.q. to s.c.	s.q. to f.c.c.
g_1	2	8
g_{21}	2	32
g_{22}	2	32
g_{31}	2	128
g_{32}	2	128
g_{33}	2	128

ed from Liu and Stanley relations.³⁰ We briefly sketch the Liu-
-Stanley arguments. First let us consider the anisotropic s.c.
lattice. The reduced susceptibility of a lattice which is com-
posed of $(N+1)$ layers with M^2 spins in each layer is given by

$$\chi(q, T) = [(N+1)M^2]^{-1} \sum_{\vec{r}_i, \vec{r}_j} \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle .$$

On differentiating with respect to g ,

$$(N+1)M^2 \left(\frac{\partial \chi}{\partial g} \right)_0 = K \sum_{\vec{\mu}_R} \sum_{z_R=1}^N \left\{ \sum_{\vec{\mu}_i} \langle s_{\vec{\mu}_i z_R} s_{\vec{\mu}_R z_R} \rangle_x \right. \\ \left. \sum_{\vec{\mu}_j} \langle s_{\vec{\mu}_j z+1} s_{\vec{\mu}_R z+1} \rangle_2 + \sum_{\vec{\mu}_i} \langle s_{\vec{\mu}_i z+1} s_{\vec{\mu}_R z+1} \rangle_2 \sum_{\vec{\mu}_j} \langle s_{\vec{\mu}_j z} s_{\vec{\mu}_R z} \rangle_2 \right\} \quad (3.26)$$

where $\langle \dots \rangle_2$ denotes the thermal average of a two-dimensional Hamiltonian. Now each of the summations inside the curly brackets is over all spins which lie in a single plane and thus each summation is exactly the reduced susceptibility of a two-dimensional lattice. Thus in the thermodynamic limit, one gets

$$\left(\frac{\partial \chi}{\partial g} \right)_0 = 2K [\chi(0)]^2 . \quad (3.27)$$

This equation is the first order correction term of the two-dimensional approximation of the three dimensional quantity $\chi(q, T)$. Similarly, they also proved relations for higher derivatives upto the third derivative. We summarize their results for the s.q. to s.c. and s.q. to f.c.c. lattices in Table 2. These relations coupled with the scaling form

$$\chi(q, T) \approx A t^{-\gamma} (\beta g / t^\phi)$$

clearly give $\phi = \gamma$.

Also using the normalization that

Table 3a. Reduced Susceptibility Expansion Coefficients b_{nl} for the s.q. to s.c. case.

n	l	b_{nl}	n	l	b_{nl}
0	0	1	5	1	$1210 \frac{2}{3}$
1	0	4	5	2	$1381 \frac{1}{3}$
1	1	2	5	3	$485 \frac{1}{3}$
2	0	12	5	4	$42 \frac{2}{3}$
2	1	16	5	5	$\frac{4}{15}$
2	2	2	6	0	$611 \frac{1}{5}$
3	0	$34 \frac{2}{3}$	6	1	$4098 \frac{2}{15}$
3	1	80	6	2	6520
3	2	32	6	3	$3761 \frac{7}{9}$
3	3	$1 \frac{1}{3}$	6	4	728
4	0	92	6	5	$34 \frac{2}{15}$
4	1	$330 \frac{2}{3}$	6	6	$\frac{4}{45}$
4	2	240	7	0	$1538 \frac{58}{315}$
4	3	$42 \frac{2}{3}$	7	1	$13112 \frac{8}{9}$
4	4	$\frac{2}{3}$	7	2	$27748 \frac{4}{15}$
5	0	$240 \frac{8}{15}$	7	3	$22855 \frac{1}{9}$

n	l	b_{nl}	n	l	b_{nl}
7	4	$7601 \frac{7}{9}$	9	4	$372997 \frac{31}{45}$
7	5	$874 \frac{2}{3}$	9	5	$118401 \frac{19}{135}$
7	6	$22 \frac{34}{45}$	9	6	$16342 \frac{38}{135}$
7	7	$\frac{8}{315}$	9	7	$749 \frac{257}{315}$
8	0	$3809 \frac{67}{105}$	9	8	$6 \frac{158}{315}$
8	1	$40234 \frac{274}{315}$	9	9	$\frac{4}{2335}$
8	2	107712	10	0	$22820 \frac{3628}{4725}$
8	3	$119472 \frac{16}{45}$	10	1	$345515 \frac{47}{2335}$
8	4	$53277 \frac{1}{3}$	10	2	$1370308 \frac{16}{21}$
8	5	$12225 \frac{19}{45}$	10	3	$2402802 \frac{302}{945}$
8	6	$874 \frac{2}{3}$	10	4	$2068551 \frac{7}{15}$
8	7	$13 \frac{1}{315}$	10	5	$918502 \frac{154}{225}$
8	8	$\frac{2}{315}$	10	6	$198700 \frac{4}{9}$
9	0	$9364 \frac{1868}{2835}$	10	7	$18700 \frac{692}{945}$
9	1	$119469 \frac{17}{315}$	10	8	$562 \frac{38}{105}$
9	2	$394827 \frac{23}{315}$	10	9	$2 \frac{2522}{2335}$
9	3	$558211 \frac{107}{315}$	10	10	$\frac{4}{14175}$

n	l	b_{nl}	n	l	b_{nl}
11	0	55317 $\frac{8046493}{14189175}$	11	6	1866900 $\frac{68}{675}$
11	1	977909 $\frac{157}{567}$	11	7	285426 $\frac{542}{945}$
11	2	4588445 $\frac{28139}{31185}$	11	8	18712 $\frac{616}{945}$
11	3	9680300 $\frac{28}{135}$	11	9	374 $\frac{518}{567}$
11	4	10409460 $\frac{34}{315}$	11	10	1 $\frac{2209}{14175}$
11	5	6037733 $\frac{427}{945}$	11	11	8 $\frac{15}{15}$

Table 3b. Reduced Susceptibility Expansion Coefficients b_{nl}
for the s.q. to f.c.c. case.

n	l	b_{nl}	n	l	b_{nl}
0	0	1	5	1	$4842 \frac{2}{3}$
1	0	4	5	2	$24501 \frac{1}{3}$
1	1	8	5	3	$52739 \frac{1}{3}$
2	0	12	5	4	$49866 \frac{2}{3}$
2	1	64	5	5	$17473 \frac{1}{15}$
2	2	56	6	0	$611 \frac{1}{5}$
3	0	$34 \frac{2}{3}$	6	1	$16392 \frac{8}{15}$
3	1	320	6	2	$113253 \frac{2}{3}$
3	2	656	6	3	$350577 \frac{7}{9}$
3	3	$389 \frac{1}{3}$	6	4	$532533 \frac{2}{3}$
4	0	92	6	5	$398216 \frac{8}{15}$
4	1	$1322 \frac{2}{3}$	6	6	$115250 \frac{22}{45}$
4	2	4544	7	0	$1538 \frac{58}{315}$
4	3	$5994 \frac{2}{3}$	7	1	$52451 \frac{5}{9}$
4	4	$2610 \frac{2}{3}$	7	2	$470871 \frac{7}{15}$
5	0	$240 \frac{8}{15}$	7	3	$1950289 \frac{7}{9}$

n	l	b_{nl}	n	l	b_{nl}
7	4	4202769 $\frac{7}{9}$	9	4	154892344 $\frac{8}{9}$
7	5	4993002 $\frac{2}{3}$	9	5	339157477 $\frac{31}{45}$
7	6	3053159 $\frac{37}{45}$	9	6	456207197 $\frac{53}{135}$
7	7	759545 $\frac{221}{315}$	9	7	372564564 $\frac{146}{315}$
8	0	3809 $\frac{67}{105}$	9	8	168266475 $\frac{43}{63}$
8	1	160939 $\frac{151}{315}$	9	9	32458605 $\frac{6611}{31185}$
8	2	1811017 $\frac{43}{45}$	10	0	22820 $\frac{3628}{4725}$
8	3	9584969 $\frac{43}{45}$	10	1	1382060 $\frac{133}{2835}$
8	4	27327480 $\frac{8}{9}$	10	2	22672635 $\frac{71}{315}$
8	5	45609776 $\frac{16}{45}$	10	3	179063707 $\frac{145}{189}$
8	6	43961545 $\frac{43}{45}$	10	4	791598100 $\frac{52}{135}$
8	7	22924237 $\frac{193}{315}$	10	5	2176311440 $\frac{46}{225}$
8	8	4966694 $\frac{182}{315}$	10	6	3813160361 $\frac{97}{135}$
9	0	9364 $\frac{1368}{2835}$	10	7	4327624997 $\frac{37}{189}$
9	1	477876 $\frac{68}{315}$	10	8	3046735819 $\frac{71}{315}$
9	2	6561420 $\frac{188}{315}$	10	9	1219450540 $\frac{23188}{31185}$
9	3	42948637 $\frac{101}{135}$	10	10	211100973 $\frac{41324}{155925}$

$$\chi(0) = \frac{d \chi(0)}{d x} = 1 . \quad (3.28)$$

we get

$$\left(\frac{\partial \chi}{\partial g} \right)_0 = A e^{-\gamma - \phi} B .$$

Using equation (3.27) we get, for $K = K_c(0)$,

$$B = 2 K_c(0) A , \quad (\text{s.q. to s.c.})$$

and

$$B = 8 K_c(0) A . \quad (\text{s.q. to f.c.c.})$$

Thus, numerically, we have,

$$B(\text{s.q. to s.c.}) = 0.848394142 \dots \quad (3.29a)$$

$$B(\text{s.q. to f.c.c.}) = 3.39357656 \dots \quad (3.29b)$$

For our analysis we have used the high-temperature series given by Harbus and Stanley,⁷⁶ Oitmaa and Enting.⁶⁹ The susceptibility series, as mentioned in Section 2.2, are obtained up to 11th and 10th order for the s.c. and f.c.c. lattices, respectively. They have been given in powers of $\tanh K$. But, for convenience, we have converted them to the form

$$\chi(g, K) = \sum_{n=0}^{10,11} a_n(g) K^n , \quad (3.30)$$

where

$$a_n(g) = \sum_{l=0}^n b_{nl} g^l$$

The coefficients so obtained are given in Table 3a,b for the s.c. and f.c.c. lattices, respectively. Many checks on our calculations of $a_n(g)$ have been carried out. We know that for $g = 1$, anisotropic lattices reduce to isotropic lattices, respectively. For this case, the coefficients $a_n(g)$ of the two lattices studied agree with their respective cases.^{31,85} For $g = 0$, both the s.c. and f.c.c. series must reduce to s.q. series.³¹ This check is also successful. Finally when $g = \infty$, the s.c. series reduces to that of linear chain, whereas the f.c.c. to body centred cubic (b.c.c.) series.^{31,85} It is found

Table 4a. Padé Estimates for the Isotropic Amplitudes for the s.c. lattice. The symbol '___' means a defective entry and n.c. means not calculated. The Estimates given here are related to the actual Estimates by the following relations. $C_2 = 4K_c^2 C_2'$, $C_3 = 8K_c^3 C_3'$, $C_4 = 16K_c^4 C_4'$, $C_5 = 32K_c^5 C_5'$, $C_6 = 64K_c^6 C_6'$.

Padé	C_2'	C_3'	C_4'	C_5'	C_6'
(1,1)	n.c.	n.c.	n.c.	---	---
(1,2)	n.c.	n.c.	n.c.	8.34509	2.82782
(2,1)	n.c.	n.c.	n.c.	9.4656×10^1	5.8627×10^2
(2,2)	1.75685	4.58772	19.6799	3.0099×10^1	1.3019×10^2
(2,3)	1.36032	3.53516	10.1069	3.36700	---
(3,2)	1.16811	1.83379	20.4840	7.1679×10^1	3.6451×10^2
(3,3)	1.60641	3.81980	13.1909	5.5753×10^1	
(3,4)	1.50436	3.65259	11.9415		
(4,3)	1.48167	3.48315	10.1643		
(4,4)	1.49333	3.51470			
(4,5)	1.47242				
(5,4)	1.48892				
(3,5)	1.49649	3.57507			
(5,3)	1.49300	3.52194			

Table 4b. Same as Table 4a, but for the f.c.c. lattice. The relations for this case are given as follows.

$$C_2 = 112K_c^2 C_2', \quad C_3 = 2336K_c^3 C_3', \quad C_4 = K_c^4 C_4', \quad C_5 = K_c^5 C_5' \\ C_6 = K_c^6 C_6'$$

Paide	C_2'	C_3'	C_4'	C_5'	C_6'
(1,1)	n.c.	n.c.	n.c.	9.1813×10^5	3.2806×10^7
(1,2)	n.c.	n.c.	n.c.	1.2625×10^6	4.4803×10^7
(2,1)	n.c.	n.c.	3.9054×10^4	1.0993×10^6	3.5043×10^7
(2,2)	0.85609	0.77103	4.3714×10^4	1.3193×10^6	4.7418×10^7
(2,3)	0.85815	0.77689	4.4463×10^4	1.3674×10^6	
(3,2)	0.85800	0.77616	4.4285×10^4	1.3489×10^6	
(3,3)	0.85644	0.77334	4.4030×10^4		
(3,4)	0.84888	0.75779			
(4,3)	0.84335	0.89603			
(4,4)	0.84610				
(5,4)	0.84298				
(1,3)				1.4582×10^6	2.7613×10^7
(3,1)			4.7084×10^4	1.4419×10^6	5.2805×10^7
(2,4)	0.86367	0.75553	3.3001×10^4		
(4,2)	0.84302	0.76891	4.3733×10^4		
(3,5)	0.84652				
(5,3)	0.84298				

that this condition is also satisfied by our series. Further tests, such as the derivative tests (upto third derivatives), are also carried out as checks on our coefficient calculations and it is found that they are satisfied.

Thus satisfied with our series, we next proceed to the analysis of the susceptibility derivatives in order to test the scaling predictions and to gain more information about the scaling function $X(x)$ near $x = 0$. The successive derivatives of χ should diverge as

$$\Xi_m \equiv \left(\frac{\partial^m \chi}{\partial g^m} \right)_0 \approx C_m t^{-(\gamma + m\phi)}, \quad t \rightarrow 0. \quad (3.31)$$

The amplitudes C_m are analysed both by the standard series methods and also by forming P.A. to

$$C_m = \left[1 - \frac{\kappa}{\kappa_c(0)} \right]^{(1+m)\phi} \left(\frac{\partial^m \chi}{\partial g^m} \right)_0,$$

obtained by taking into account the fact that $\phi = \gamma$ in (3.31). The results are presented in Table 4 for the two lattices. Considering normalization conditions, we can easily see from equation (3.31) that

$$C_0 = A, \quad C_1 = AB, \quad (3.32)$$

and hence

$$C_m = AB^m \left(\frac{d^m X}{d x^m} \right)_0. \quad (3.33)$$

Since the scaling function $X(x)$ is universal, the ratio of the amplitudes

$$R_m = \frac{C_{m-1} C_{m+1}}{C_m^2} = \frac{\Xi_{m-1} \Xi_{m+1}}{\Xi_m^2}, \quad m \geq 1, \quad (3.34)$$

are predicted to be universal. P.A. and ratio methods are used

Table 5a. Pade Estimates for the Universal Ratios for the s.c. lattice. The numbers are the values of the P.A. evaluated at $K = K_c(0)$. The symbol '—' means a defective entry, n.c. means not calculated.

Pade	R_1	R_2	R_3	R_4	R_5
(1,1)	n.c.	n.c.	n.c.	1.3781	1.3369
(1,2)	n.c.	n.c.	n.c.	0.4392	0.2264
(2,1)	n.c.	n.c.	n.c.	—	—
(2,2)	1.7918	1.4862	1.2617	1.1791	1.1238
(2,3)	1.0650	1.4617	1.4402	1.9235	4.6123
(3,2)	2.4663	1.4605	1.4136	1.6009	1.9174
(3,3)	1.7242	1.6715	1.2996	1.2633	
(3,4)	1.6667	1.4570	1.2521		
(4,3)	1.6554	1.4557	1.2470		
(4,4)	1.6718	1.4727			
(3,5)	1.6729	1.5112			
(5,3)	1.6911	1.5192			
(5,4)	1.6712				
(4,5)	1.6712				

Table 5b. Pade Estimates for the Universal Ratios for the
f.c.c. lattice evaluated at $K = K_c(0)$.

Pade	R_1	R_2	R_3	R_4	R_5
(1,1)	n.c.	n.c.	1.0000	1.0000	1.0000
(1,2)	n.c.	n.c.	0.2095	—	0.2093
(2,1)	n.c.	n.c.	—	2.5596	—
(2,2)	0.9321	1.0033	0.2748	—	0.2738
(2,3)	0.9067	0.9155	0.2073	0.3074	
(3,2)	0.8994	0.9100	6.4398	9.7258	
(3,3)	0.9414	0.8973	2.4557		
(3,4)	0.9512	0.9073			
(4,3)	0.9508	0.9054			
(4,4)	0.9490				
(3,5)	0.9456				
(5,3)	0.9475				

Table 6. Overall Estimates for the Universal Amplitude Ratios
 R_m .

Ratio	f.c.c.	s.c.	Adopted mean	Mean- field value	Spherical model
R_1	1.6703	1.6715	1.6709	2	1.5
R_2	1.4783	1.4718	1.4755	1.5	1.333 ...
R_3	1.2914	1.2924	1.2919	1.333 ...	1.25
R_4	1.2599	1.2410	1.2505	1.25	1.2
R_5	1.1243	1.1402	1.1323	1.2	1.666 ...

to calculate R_m . The results of our analysis are displayed in Table 5, for both the s.c. and f.c.c. lattices, for the values of $m = 1$ to $m = 5$ evaluated at $K = K_c(0)$. We also find that for R_m 's, on the whole, the standard methods give consistent results except for the f.c.c. case for $m > 1$, which for unexplained reasons is badly behaved. Accordingly, we have omitted it in our analysis. The overall estimates for the two lattices and the mean-field theory values are listed together in Table 6. The recently calculated values for the spherical model are also shown.⁸⁶ It can be seen clearly that the values for the Ising models lie between those of the mean-field and spherical model values. A similar behaviour was found in the parallel case of spin-space anisotropy.^{59,60} Our confidence limits based on overall analysis are 1,1,2,3 and 5% in the amplitudes R_1 to R_5 respectively. It is evident that the central estimates for the amplitudes ratios, for the two lattices under study, match each other within at most 1%. Hence the scale-factor universality of the scaling function is confirmed within these limits. (Having known so many of the input parameters exactly, we should have expected the results to be more accurate than this, but our experience shows that the analysis is difficult because of the high value of the crossover exponent $\phi = 7/4$).

From the mean adopted values of the universal ratio amplitudes R_1 to R_5 , one can get an expansion of the scaling function $X(x)$. Using the normalization (3.28) and the expression (3.34), $X(x)$ can be expanded near $x = 0$ as

$$X(x) = 1 + x + \frac{R_1}{2} x^2 + \frac{R_1^2 R_2}{3} x^3 + \dots$$

We get

$$X(x) = 1 + x + 0.83545 x^2 + 0.6866 x^3 + 0.5467 x^4 + 0.4355 x^5 + 0.3273 x^6 + \dots \quad (3.35)$$

with the extrapolation uncertainties of about 1, 1.7, 3, 5 and 8% in the coefficients x^2 to x^6 , respectively. The above representation of the scaling function $X(x)$ is valid for $x \ll 1$.

In the vicinity of the critical value \dot{x} , the scaling function should have a form⁵⁸

$$X(x) \approx \dot{X} \left(1 - \frac{x}{\dot{x}} \right) . \quad (3.36)$$

Preliminary estimates of \dot{x} and \dot{X} are obtained by forming direct P.A. to the six-term series of $X(x)$. Thus we get, taking into account the singularity of $X(x)$ at \dot{x} ,

$$\dot{x} = 1.334 \quad , \quad \dot{X} = 1.071 .$$

Thus so far, we have obtained the values of \dot{x} and \dot{X} by considering the $g = 0$ behaviour of the susceptibility. In the next Chapter, we look at the detailed behaviour of the model for $g \neq 0$.

Anisotropic Behaviour

4.1. Introduction

So far, we have seen in the preceding Chapter that the scaling theory holds good for the case of small g in the limit $g \rightarrow 0$. In this Chapter, we study the behaviour of the model for g small, but not equal to zero. We need small values of g because the scaling theory does not apply for larger g , say $\gtrsim 10^{-2}$. However, for very small values of g , one needs longer series for a reliable analysis. Therefore, for the crossover scaling analysis, there is a typical window for the values of g . An estimate of this range can be made by making a scaling hypothesis for the coefficients $a_n(g)$. Following PJF,⁵⁸ we have

$$a_n(g) \approx a_n(0) F(ng^{1/\phi}), \quad n \rightarrow \infty, \quad g \rightarrow 0 \quad (4.1)$$

$$F(0) = 1.$$

This predicts, e.g., that the sequence

$$\dot{\omega}_n = g^{1/\phi} \left[\frac{n f_n(g) K_c(0)}{n + \nu - 1} - 1 \right],$$

where,

$$r_n(g) = a_n(g) / a_{n-1}(g) \quad ,$$

should vary as

$$\dot{\omega}_n \approx \dot{\omega} + (\dot{\gamma} - \gamma) / n g^{1/\phi} \quad , \quad n g^{1/\phi} \rightarrow \infty \quad .$$

Applying this method to our model, we find that the ranges of g amenable to analysis are $0.01 \lesssim g \lesssim 0.08$ and $0.005 \lesssim g \lesssim 0.02$ for the s.c. and f.c.c. lattices, respectively. This is in general agreement with the previous work of Harbus and Stanley,⁷⁶ who obtained similar ranges by a different method.

Having decided on the values of g to work with, the next step is to estimate the critical temperature $K_c(g)$. The critical point shifts $\dot{\omega}$ are calculated in order that the location of the singularity, x , in the scaling function can be determined. Critical amplitudes $A(g)$ can then be estimated by standard methods. Having obtained $A(g)$, one can find A and X . The constants x and X are universal while the scale factors $A, B, \dot{\omega}$ and A_∞ are non-universal.

In the coming Sections, we will give a detailed report on the methods used and the results obtained, for all these parameters except A and B which were already obtained in Section 3.2.

4.2. Estimation of Critical Points and Critical Amplitudes

Generally, one may believe that there is no special problem involved in the estimation of $T_c(g)$ from the susceptibility series at fixed g . However, standard methods have been found to depend rather heavily for their success on a simple-

Fig. 4a

- | | | |
|----------------|----------------|----------------|
| (a) $g = 0.01$ | (d) $g = 0.04$ | (g) $g = 0.07$ |
| (b) $g = 0.02$ | (e) $g = 0.05$ | (h) $g = 0.08$ |
| (c) $g = 0.03$ | (f) $g = 0.06$ | (i) $g = 0.09$ |

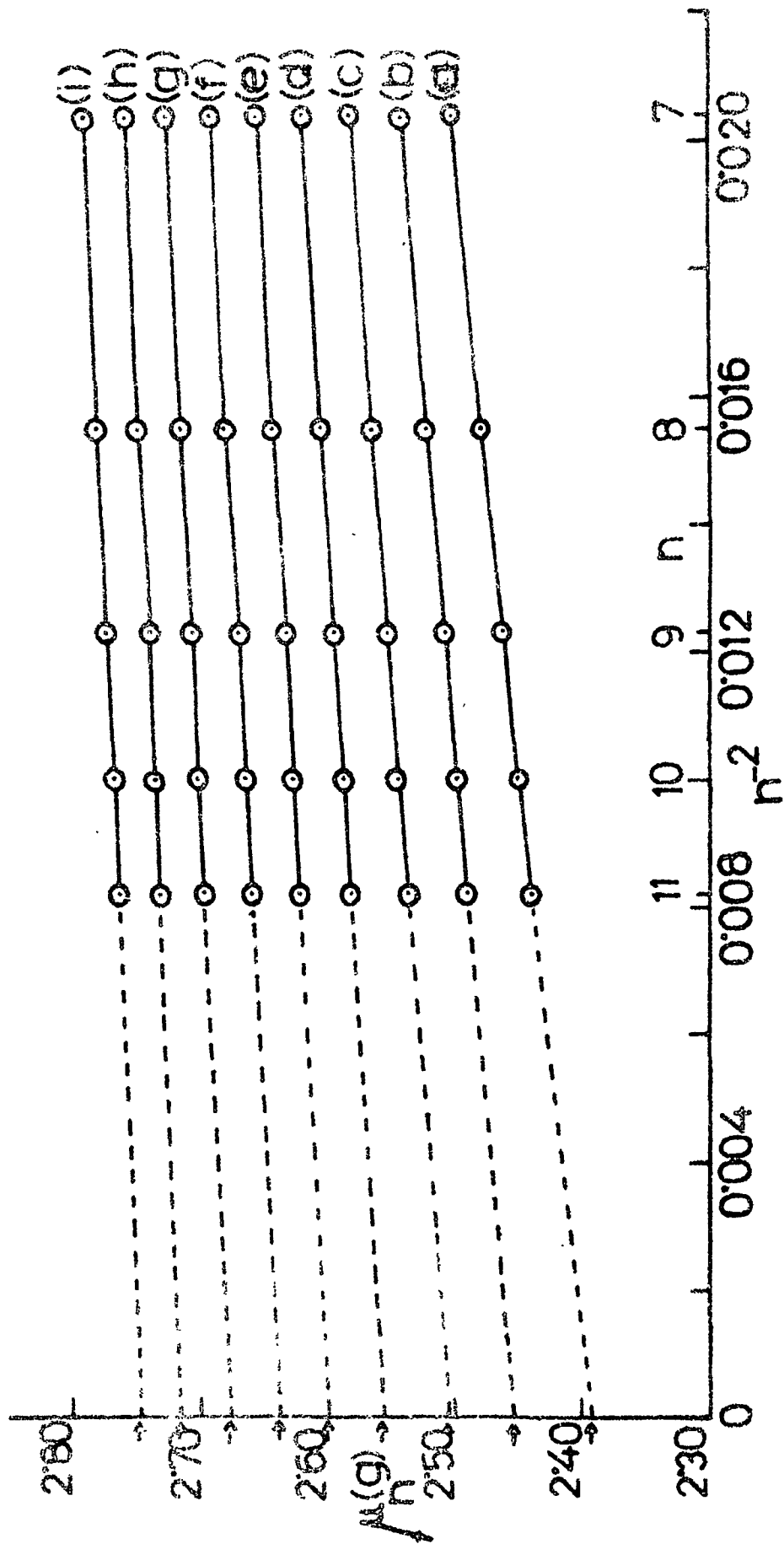
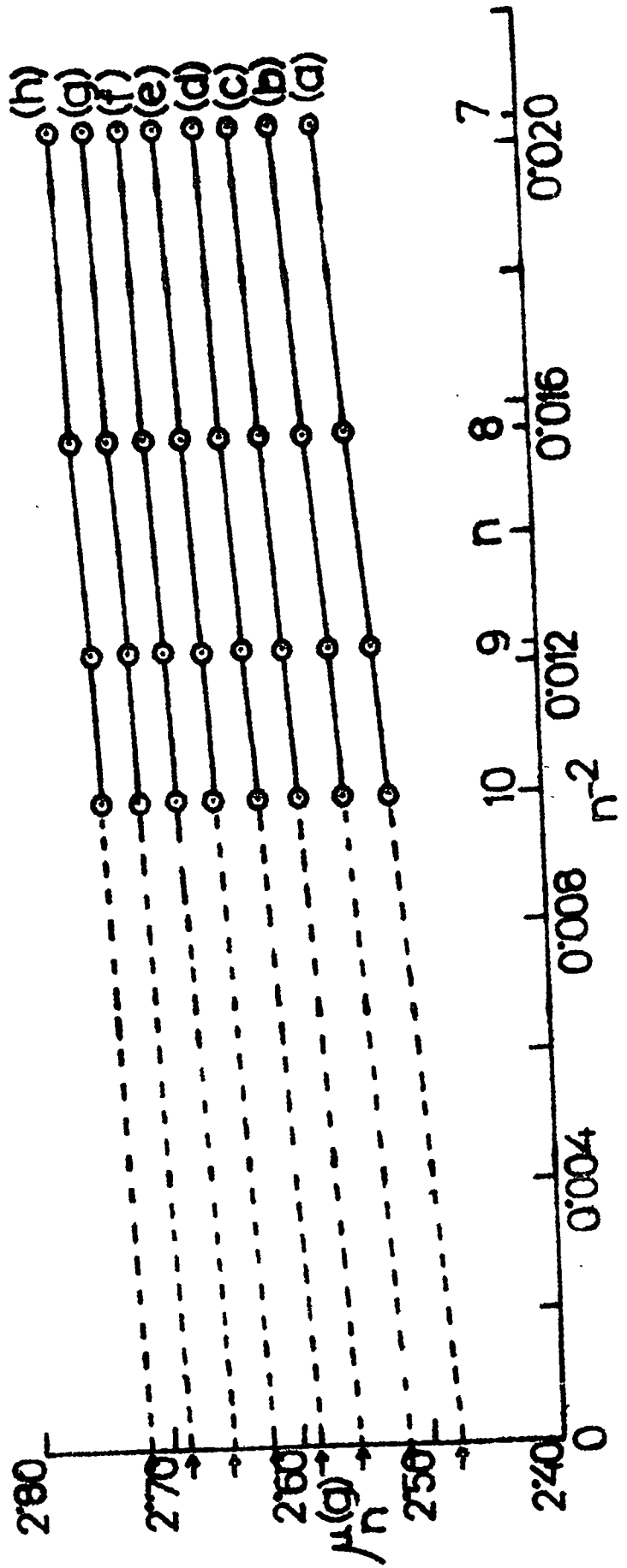


Fig. 4b

(e) $g = 0.014$
 (f) $g = 0.016$
 (g) $g = 0.018$
 (h) $g = 0.020$

(a) $g = 0.006$
 (b) $g = 0.008$
 (c) $g = 0.010$
 (d) $g = 0.012$



-power-law behaviour of $\chi(g, T)$. The difficulty here lies in the fact that the susceptibility at small g changes over from one power law form to another at a crossover temperature which lies very close to $T_c(g)$. Failure to recognize this point may lead to unusual behaviour, e.g., the dependence of γ on g ,^{69,70} which is really an artifact of the shortness of the series.⁷¹ On the other hand, if g is large enough, the estimation of $T_c(g)$ by straightforward methods can be trusted.

Before proceeding further, we comment on the assignment of the "known" parameters; because the final values of various parameters will be particularly sensitive to the assumed value of γ . For the value of γ we have chosen 1.75 (see Section 1.1). The value of $\gamma = 1.25$ corresponds to the value of γ for the three-dimensional Ising model. (Very recently Chen, Fisher and Nickel⁸⁷ obtained $\gamma = 1.238$ in their study of the Ising model, using a series of 21 terms. But since our series are shorter (upto 10th and 11th order) and their analysis gives $\gamma = 1.25$, we have chosen this value for consistency.)

Now to estimate $K_c(g)$, apart from the standard methods,²¹ following PJF, we extrapolate the sequence

$$\mu_n(g) = \left(\frac{n+\epsilon}{n+\epsilon+\gamma-\gamma} \right) \frac{f_n(g)}{f_n(0)}, \quad (4.2)$$

versus n^{-1} . We have varied the shift ϵ in order to check the consistency and to improve the overall smoothness of the sequence. It is expected that (4.2) should approach $K_c(g)$ linearly in the variable n^{-2} as $n \rightarrow \infty$. This is indeed verified as can be seen from Figures 4a,b, where we present the plots of $\mu_n(g)$ versus n^{-2} for various values of g for the s.c. and f.c.c. lattices, respectively.

Fig. 5a

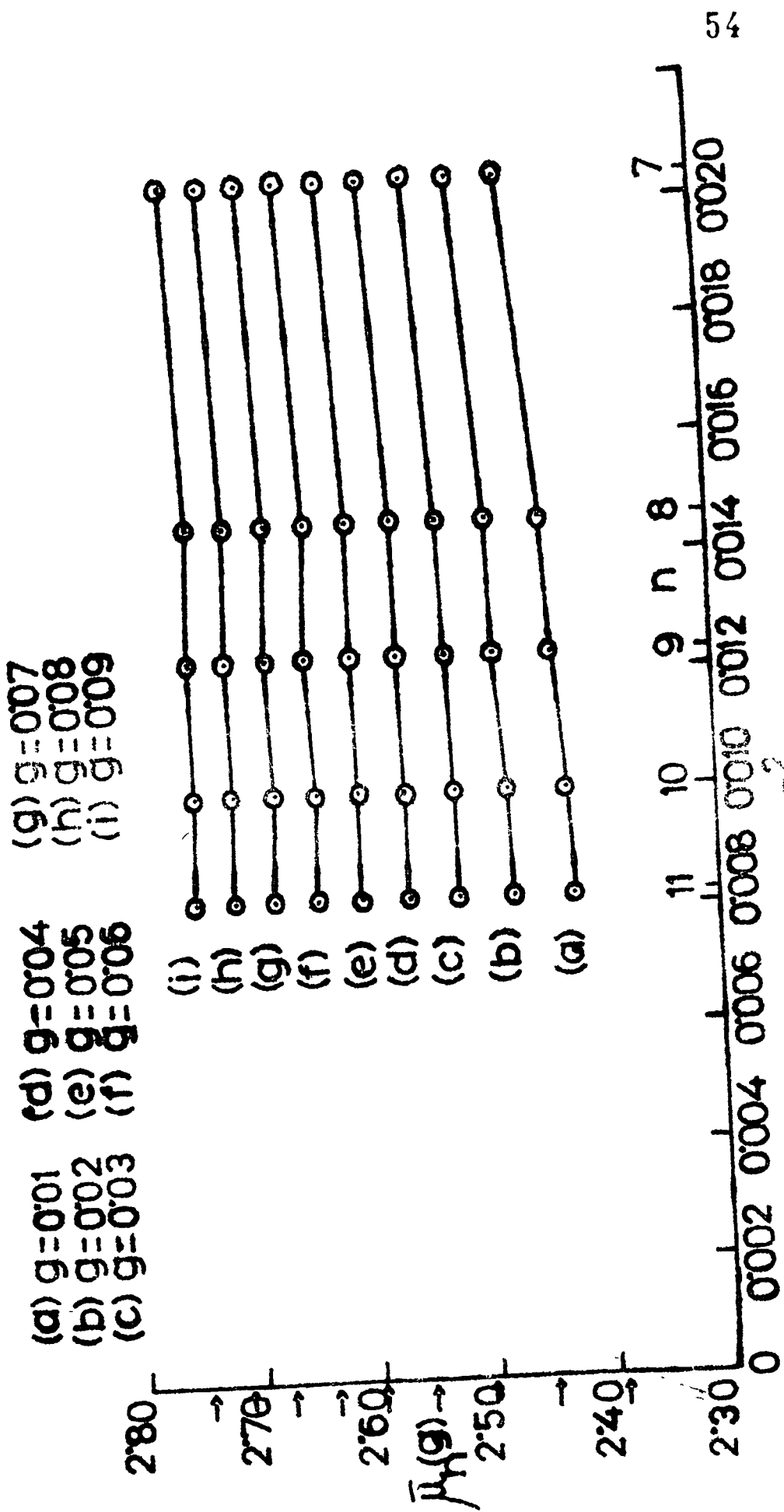


Fig. 5b

(a) $g = 0.0006$
 (b) $g = 0.0008$
 (c) $g = 0.0010$
 (d) $g = 0.0012$

(e) $g = 0.0014$
 (f) $g = 0.0016$
 (g) $g = 0.0018$
 (h) $g = 0.0020$

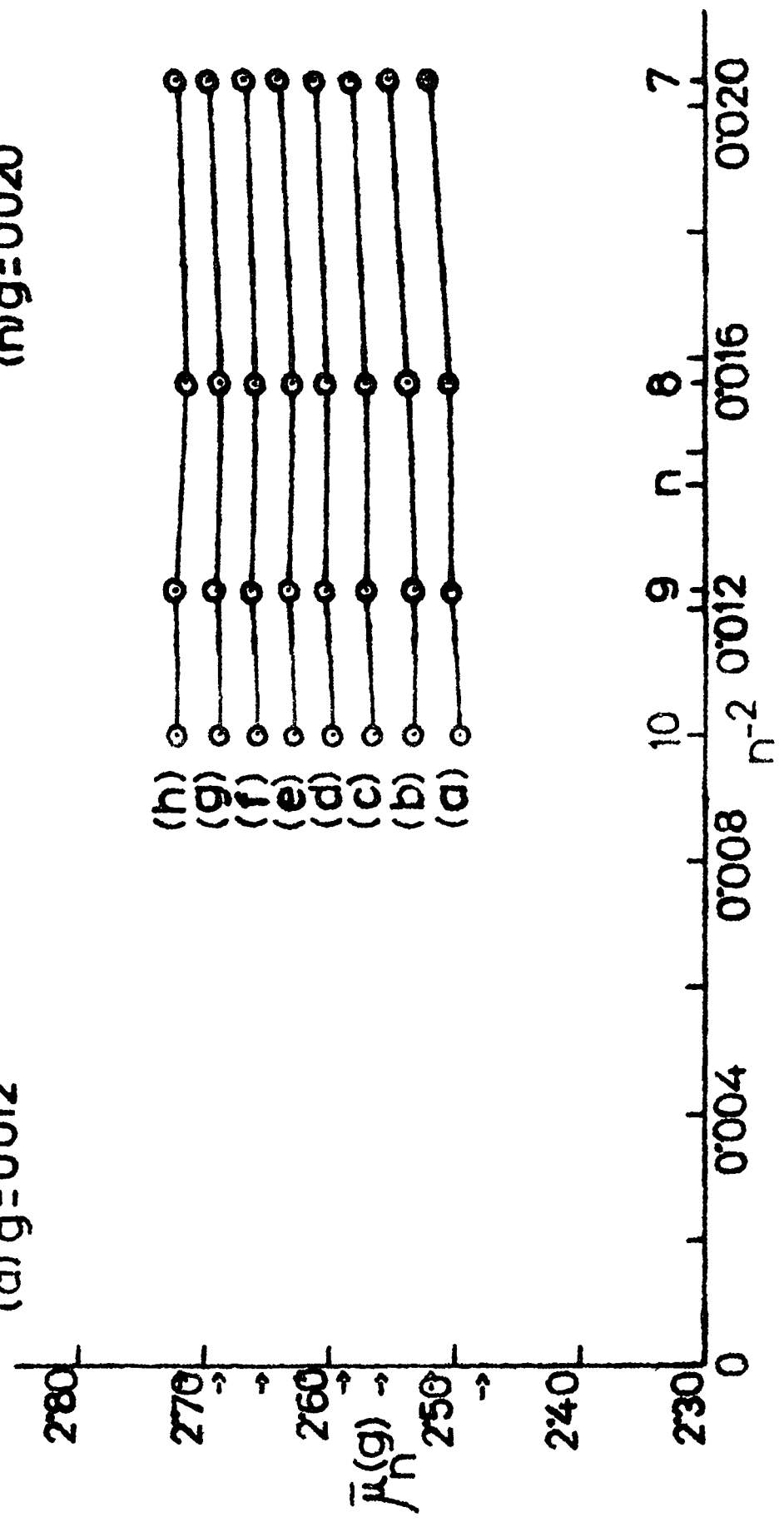


Table 7. Estimates of Critical Temperatures $K_c(g)$ for various values of g , for the s.c. and f.c.c. lattices. Extrapolation uncertainty is about 0.2%.

f.c.c.		s.c.	
g	$K_c(g)$	g	$K_c(g)$
0.006	0.40355	0.01	0.41806
0.008	0.39730	0.02	0.40766
0.010	0.39093	0.03	0.39872
0.012	0.38595	0.04	0.39124
0.014	0.38110	0.05	0.38476
0.016	0.37636	0.06	0.37893
0.018	0.37202	0.07	0.37341
0.020	0.36792	0.08	0.36846
		0.09	0.36390

Table 8. Estimates of the Critical Amplitudes $\dot{A}(g)$ for various values of g for the s.c. and f.c.c. lattices. Extrapolation uncertainty is about 4%.

f.c.c.		s.c.	
g	$\dot{A}(g)$	g	$\dot{A}(g)$
0.006	1.985	0.01	2.495
0.008	1.861	0.02	2.135
0.010	1.706	0.03	1.878
0.012	1.647	0.04	1.722
0.014	1.5755	0.05	1.624
0.016	1.505	0.06	1.543
0.018	1.4535	0.07	1.469
0.020	1.4055	0.08	1.4175
		0.09	1.378

In addition, conventional methods for finding the critical temperatures, e.g., using the sequences

$$\bar{\mu}_n(g) = \left(\frac{n+\epsilon}{n+\epsilon+\gamma-1} \right) \mu_n(g) \quad , \quad (4.3)$$

have also been used. These are found to show oscillations owing to the loose-packed nature of the s.q. lattice. The plots versus n^{-2} are presented in Figures 5a,b for the s.c. and f.c.c. lattices, respectively. In (4.2) these oscillations are cancelled to a large extent due to the presence of the ratio $\frac{\mu_n(g)}{\mu_n(0)}$. Extrapolations of the plots of $\mu_n(g)$ versus n^{-2} allow us to estimate $K_c(g)$ to an accuracy of about a conservative 0.2%. Our estimates of $K_c(g)$ based on overall analysis are listed in Table 7 for both the lattices.

Knowing the values of $K_c(g)$, we can now determine the critical amplitudes. This is done by using the conventional ratio methods based on the extrapolation of

$$\left[\dot{A}(g) \right]_n = a_n(g) \left[K_c(g) \right]^n / \binom{n+\gamma-1}{n} \quad ,$$

versus n^{-1} which are found to work well for both the cases. Our estimates for $\dot{A}(g)$ are listed in Table 8. Uncertainties in the amplitudes are about 4% and come mainly from those in $K_c(g)$.

Thus we have estimated the critical points and the amplitudes. In the coming Section we will proceed with the calculations of ω_{eff} from $K_c(g)$ and hence the shift amplitude. Finally from these values we will calculate x_c .

Table 9. Critical Point Shifts for the s.c. and f.c.c. lattices. Uncertainties in the last place are indicated in the brackets.

f.c.c.		s.c.	
g	$w_{\text{eff}}(g)$	g	$w_{\text{eff}}(g)$
0.006	1.568 (50)	0.01	0.7134 (390)
0.008	1.554 (40)	0.02	0.7008 (260)
0.010	1.569 (40)	0.03	0.7063 (200)
0.012	1.555 (30)	0.04	0.7060 (170)
0.014	1.550 (30)	0.05	0.7030 (145)
0.016	1.551 (30)	0.06	0.6994 (130)
0.018	1.547 (25)	0.07	0.6972 (120)
0.020	1.544 (20)	0.08	0.6840 (110)
		0.09	0.6898 (100)

Fig. 6a

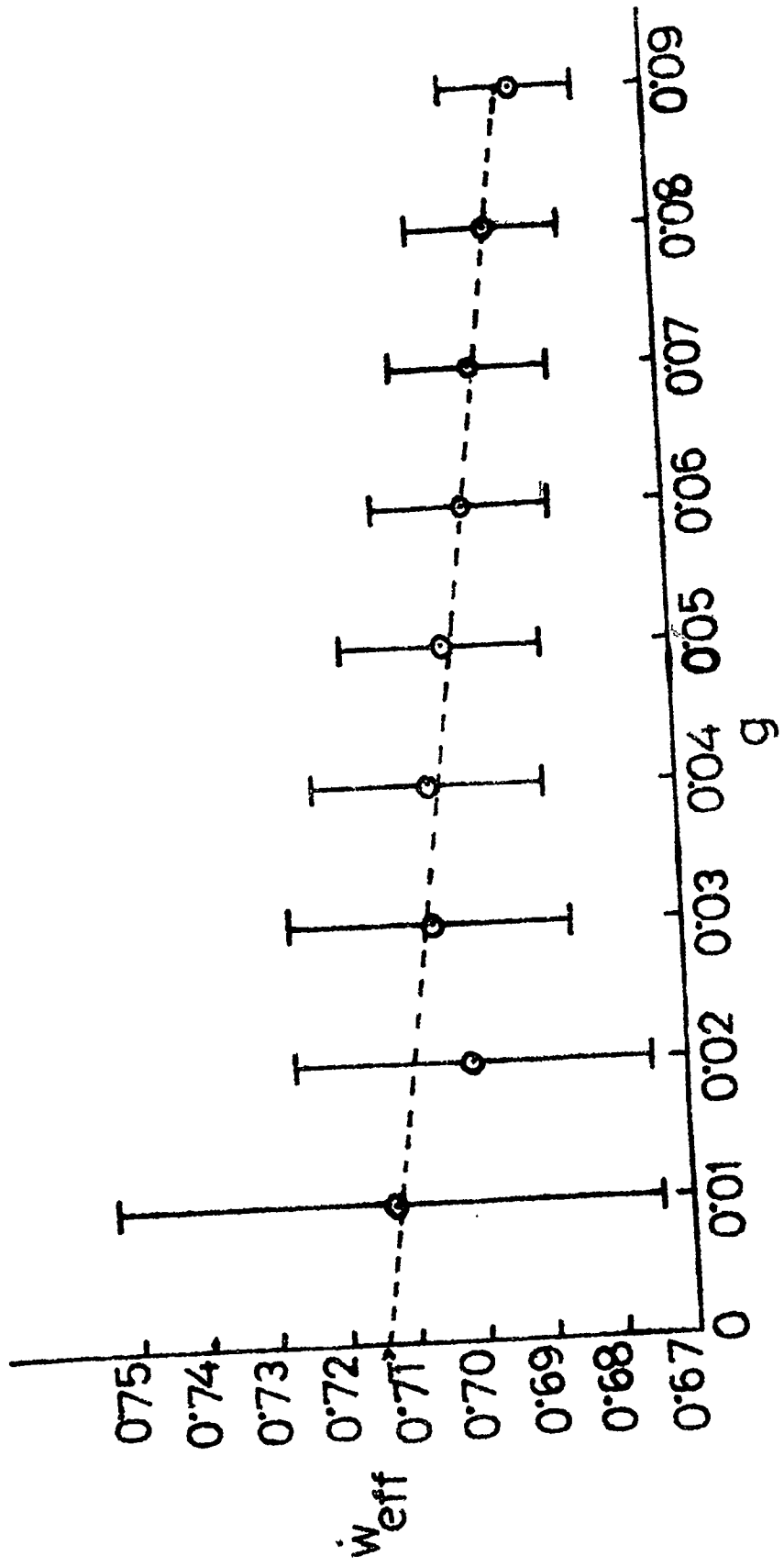
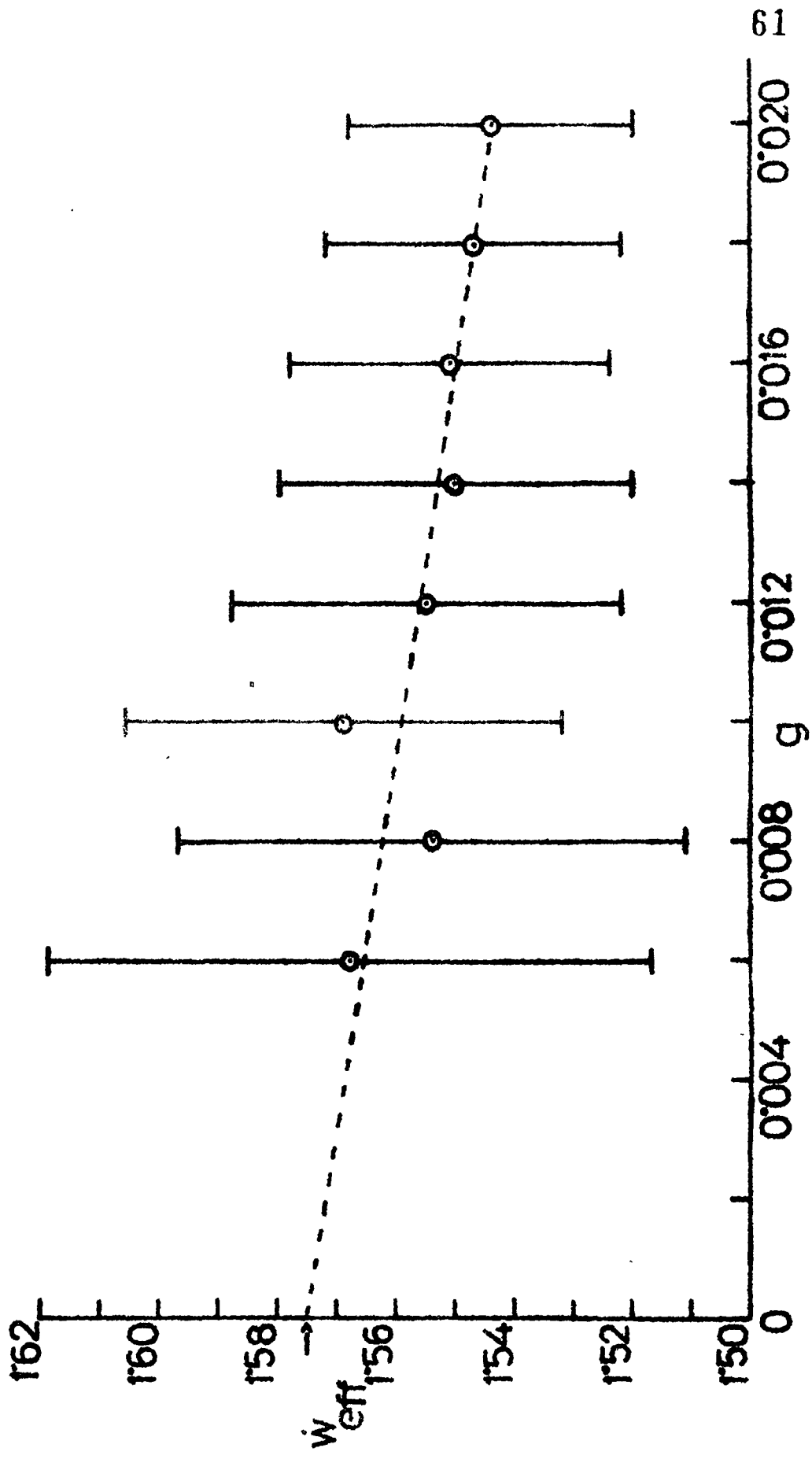


Fig. 6b



4.3. Estimation of $\dot{\omega}$ and \dot{x}

In the previous Section, we have calculated the values of the critical temperatures $K_c(g)$ for different values of g and also the values of the critical amplitudes $\dot{A}(g)$ for both the lattices under study. It is believed⁵³ that $\dot{K}_c(g)$ varies linearly with $g^{4/\phi}$ over a wider range than its inverse which is $k_B T_c(g)/J$. To enable the extrapolation to be carried out to small g , we define⁵⁸

$$\dot{\omega}_{\text{eff}}(g) = g^{-1/\phi} \left[\frac{K_c(0) - K_c(g)}{K_c(0)} \right]. \quad (4.4)$$

Here we have accepted $\psi = \phi$ and plotting $\log [K_c(0) - K_c(g)]$ versus $\log g$ confirms this.⁷⁶ Table 9 gives our calculated values of $\dot{\omega}_{\text{eff}}(g)$ for both s.c. and f.c.c. lattices. These are seen to depend weakly on g . To obtain $\dot{\omega}$, we extrapolate $\dot{\omega}_{\text{eff}}(g)$ versus g and g . In both the cases, we get similar results. In Figures 6a,b we represent graphs of $\dot{\omega}_{\text{eff}}(g)$ versus g for both s.c. and f.c.c. lattices from which we conclude that,

$$\dot{\omega} = 0.715 \pm 0.025 \quad (\text{s.c.}) \quad (4.5a)$$

$$\dot{\omega} = 1.575 \pm 0.055 \quad (\text{f.c.c.}) \quad (4.5b)$$

The uncertainties in $\dot{\omega}$ reflect those mainly present in $K_c(g)$. The values of $\dot{\omega}$ are non-universal, but using the definition (2.13) and the non-universal values of θ from (3.29) we can, in each case, determine the universal parameter x .

$$\dot{x} = 1.526 \pm 0.090 \quad (\text{s.c.}) \quad (4.6a)$$

$$\dot{x} = 1.533 \pm 0.090 \quad (\text{f.c.c.}) \quad (4.6b)$$

It is found that the central estimates agree with each other

Table 10. Estimates of the Anisotropic Amplitudes $\dot{A}_{eff}(g)$ for the s.c. and f.c.c. lattices. Uncertainties in the last place are indicated in the brackets.

f.c.c.		s.c.	
g	$\dot{A}_{eff}(g)$	g	$\dot{A}_{eff}(g)$
0.006	0.4602 (270)	0.01	0.6693 (470)
0.008	0.4684 (250)	0.02	0.6982 (440)
0.010	0.4577 (250)	0.03	0.6896 (450)
0.012	0.4655 (250)	0.04	0.6865 (450)
0.014	0.4653 (300)	0.05	0.6900 (430)
0.016	0.4618 (260)	0.06	0.6907 (440)
0.018	0.4612 (250)	0.07	0.6872 (430)
0.020	0.4596 (250)	0.08	0.6888 (450)
		0.09	0.6926 (450)

to about 0.5%, and hence the scale-factor universality is very well satisfied. For further work, from the above two values, we adopt the mean of the central estimates as the universal value, viz.,

$$\bar{x} = 1.530 .$$

It is to be noted that we have mostly avoided using the Pade method for the $g \neq 0$ analysis as this was already done by Harbus and Stanley^{76b} in their study of this model. Their aim was mainly to test the double power-law predictions. However, on using their Figures 2a and 3, we estimate the values of $\omega(A_\infty)$ from their analysis to be consistently higher (lower) than our central estimates for the two models, but within our confidence limits.

The coming Section deals with the estimation of A and X .

4.4. Estimation of Critical Amplitudes A_∞ and X

From the values of $\dot{A}(g)$ obtained in Section 4.2, we form

$$\dot{A}(g)_{\text{eff}} = \dot{A}(g) g^{(\gamma - \bar{\gamma})/\phi},$$

which are again found to have a weak dependence on g . The values of $\dot{A}(g)_{\text{eff}}$ for various values of g are listed in Table 10. To obtain A_∞ from $\dot{A}(g)_{\text{eff}}$, we extrapolated them to $g = 0$ against g and $g^{1/\phi}$ to give

$$A_\infty = 0.690 \pm 0.040 \quad (\text{s.c.}) \quad (4.7a)$$

$$A_\infty = 0.462 \pm 0.025 \quad (\text{f.c.c.}) \quad (4.7b)$$

Fig. 7a

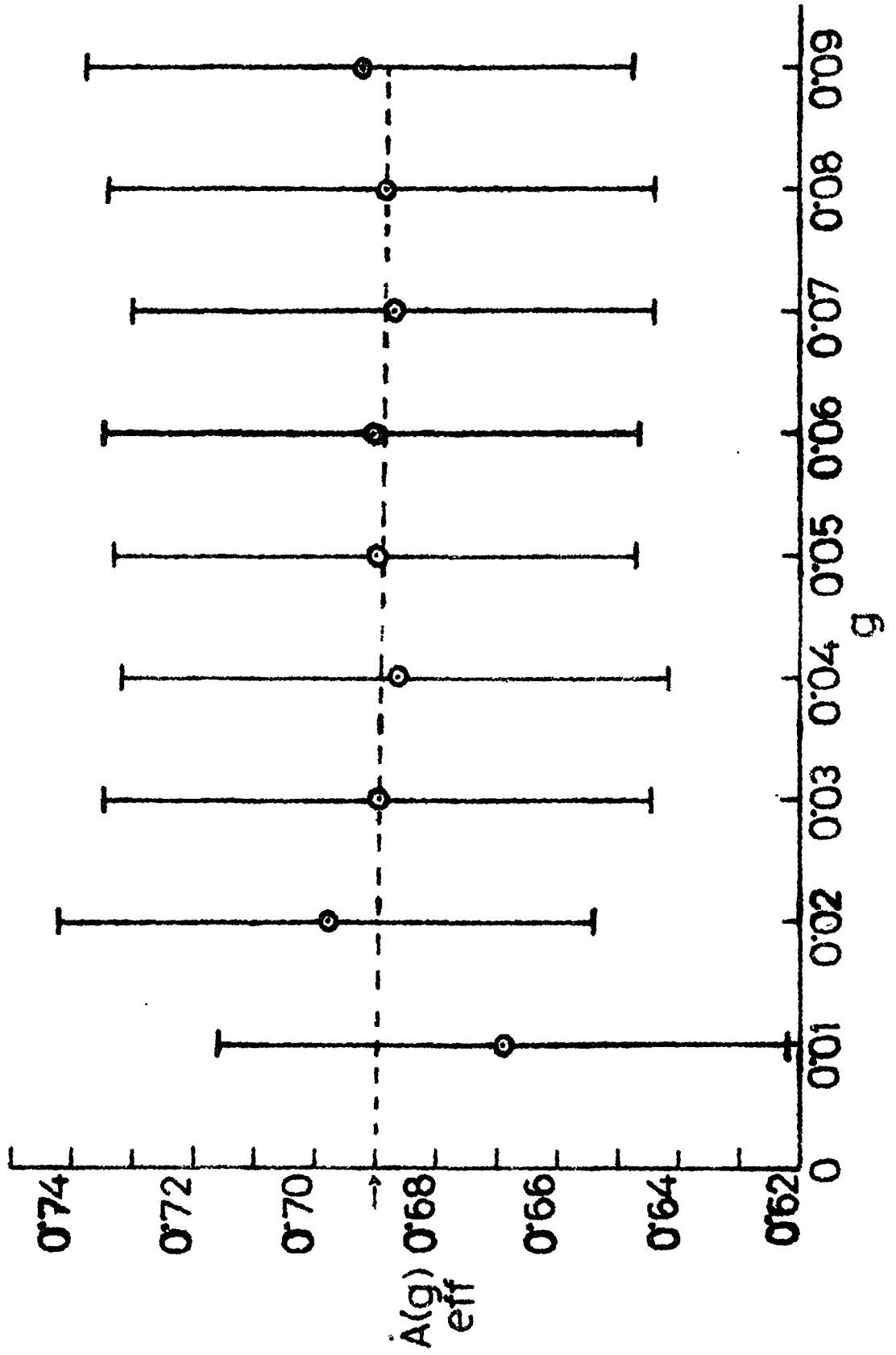
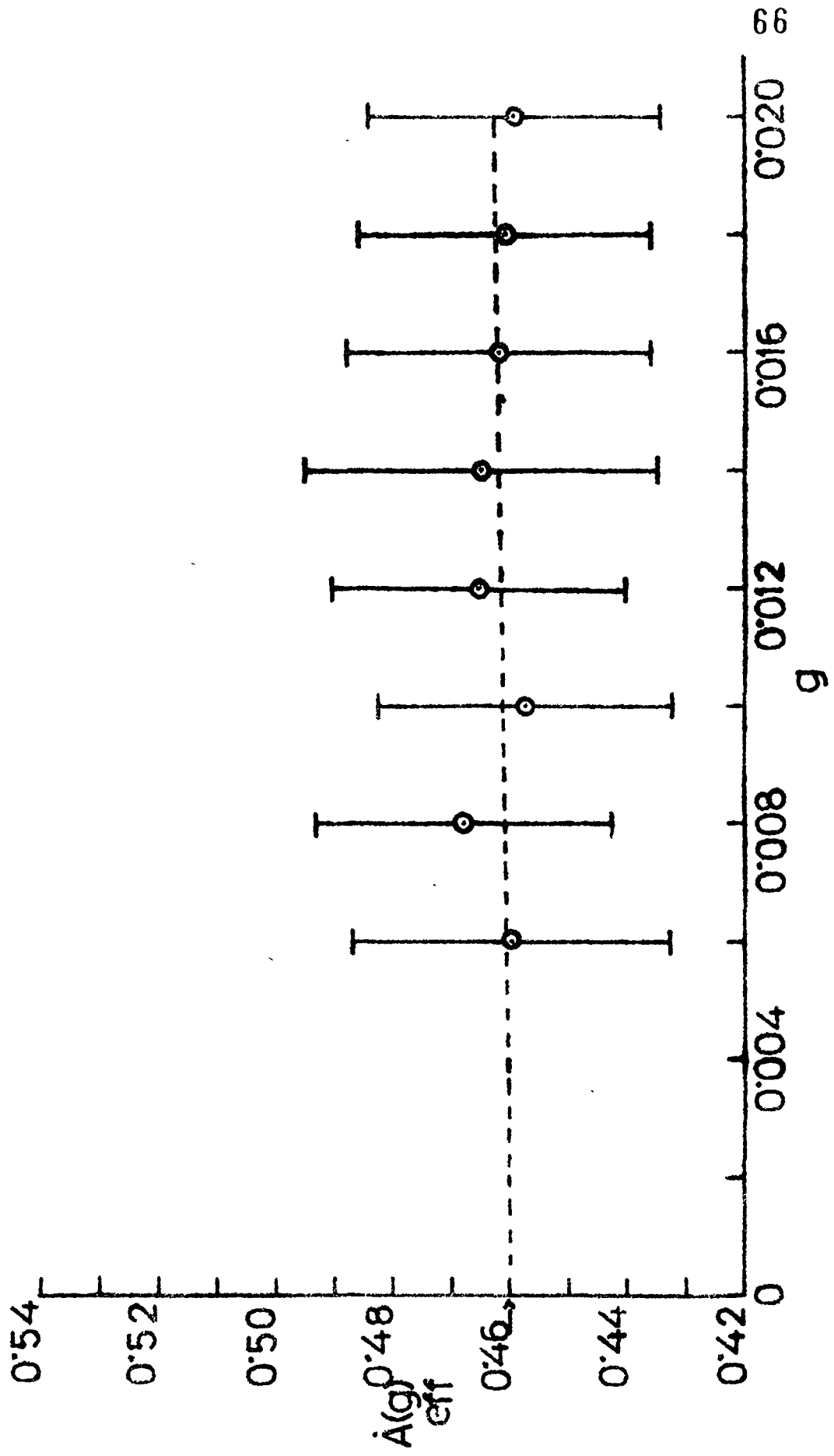


Fig. 7b



In Figures 7a,b, we show these extrapolations versus g for the two lattices studied. Again the uncertainties in the values of A_∞ reflect those in $K_c(g)$. Once again, we can test the universality by evaluating \dot{X} using the separate non-universal constants from (4.7), $\dot{\omega}$ from (4.5) and A from (3.25), through the relation [equation (2.15)]

$$\dot{X} = A_\infty \dot{\omega}^{(\gamma-\gamma')} \phi^{\gamma'} / A$$

The results for the two independent calculations are

$$\dot{X} = 1.220 \pm 0.070 \quad (\text{s.c.}) \quad (4.8a)$$

$$\dot{X} = 1.212 \pm 0.070 \quad (\text{f.c.c.}) \quad (4.8b)$$

We note that the central estimates of \dot{X} for the two lattices agree with each other within 0.7%. Hence, we conclude that the scale-factor universality of the scaling function is very well satisfied. For further work, we take the universal value of \dot{X} to be 1.216. In passing we remark that these values agree within 10 - 12% with the crude estimates in Section 3.2 obtained from the $g = 0$ analysis. Of course, the estimates obtained in the present work are the result of a much more detailed ($g \neq 0$) analysis and are believed to be more accurate.

In summary, we have examined the crossover scaling function for the quasi-two-dimensional Ising model in detail, for small but finite g in the scaling regime, and have confirmed the scale-factor universality of the critical point shift and amplitude.

We will now turn to the construction of approximants for the full scaling function in the next Chapter.

Scaling Functions and the Effective Exponent

5.1. Introduction

To recapitulate, we have discussed the ferromagnetic quasi-two dimensional Ising model with the anisotropic exchange coupling for the s.c. and f.c.c. lattices. We have analyzed the high-temperature series expansions for $\chi(q, T)$, in terms of the extended scaling theory

$$\chi(q, T) \approx A t^{-\gamma} X(Bq/t^\phi), \quad (5.1)$$

with

$$t = [T - T_c(0)] / T_c(0). \quad (5.2)$$

The non-universal parameters A , B and $K_c(0)$ were discussed in Section 3.2. They were obtained exactly from previously known results. We have obtained an expansion for $X(x)$ to order x^6 and in the process demonstrated the universality of the available coefficients. We have also studied the "large"- x behaviour and, in particular, have checked the universality of \dot{x} and \ddot{X} defined in the asymptotic form

$$X(x) \approx \dot{X} \left(1 - \frac{x}{\dot{X}}\right)^{-\dot{\gamma}}, \quad x \rightarrow \dot{X} \quad (5.3)$$

In order to determine $X(x)$ more precisely and to interpolate between the small x and large x behaviour, we write

$$X(x) = P(x/\dot{X}) / [1 - (x/\dot{X})]^{\dot{\gamma}}, \quad (5.4)$$

where,

$$P(0) = 1, \quad P(1) = \dot{X} \quad (5.5)$$

By construction, $P(z)$ is expected to be a rather smooth function of its argument. It is determined as a power series in $z (= x/\dot{X})$ to order z^6 using the known power series for $X(x)$ in **equation 3.35**. It is natural to form two-point P.A. to construct a representation of $P(z)$ valid over the whole range from $z = 0$ to $z = 1$.

Before presenting the approximants, we note that the values of the universal parameters \dot{x} and \dot{X} we have adopted are

$$(i) \quad \dot{x} = 1.334, \quad \dot{X} = 1.071, \quad (5.6)$$

which come from the $g \approx 0$ analysis, see Section 3.2. The values from $g \neq 0$ analysis (see Sections 4.3 and 4.4) are

$$(ii) \quad \dot{x} = 1.530, \quad \dot{X} = 1.216, \quad (5.7)$$

In the next Section, we will deal with the scaling functions corresponding to the above two cases.

Table 11. Coefficients of Padé Approximants for various $P(z)$ for $\bar{X} = 1.334$ and $\bar{X} = 1.071$.

Coefficients	(2,5)	(3,4)	(5,2)	(2,4)	(3,3)	(4,2)	(4,3)
P_0	1	1	1	1	1	1	1
P_1	2.5194	-1.7924	2.8703	-3.0335	-2.9893	-3.111	-0.90575
P_2	-2.5858	10.491	-3.8981	-2.1306	-1.6805	-2.1715	7.9044
P_3		9.1866	-0.39419		0.32755	-0.06080	7.8061
P_4			0.14933			-0.02011	0.37986
P_5			-0.07148				
q_0	1	1	1	1	1	1	1
q_1	2.4354	-1.8764	2.7863	-3.1115	-3.0733	-3.2010	-0.98965
q_2	-2.7659	10.6761	-4.1076	-1.8442	-1.3978	-1.8781	7.9628
q_3	0.27288	8.2246		0.05930	0.35044		7.1435
q_4	-0.13262	-0.38832		0.01436			
q_5	0.06191						

5.2. Scaling Function Case (i)

We have studied the diagonal and near-diagonal approximants to $P(z)$, viz., $[2,2]$, $[2,3]$, $[3,2]$, $[2,4]$, $[4,2]$, $[3,3]$, $[3,4]$ and $[4,3]$. Their values are given in Table 11. By studying these P.A. in detail, we find that many of the approximants except $[3,4]$ and $[4,3]$ show a pole in the range $0 \leq z \leq 1$. Presumably, the only singularity of $X(x)$ should be at x , so $P(z)$ should be smooth. So we reject all the P.A. except $[3,4]$ and $[4,3]$ as unsuitable. These two P.A. agree with each other within 1%. We have chosen the $[4,3]$ approximant for further work. The value of $P(z)$ obtained from the $[4,3]$ approximant is

$$P(z) = \frac{1 - 0.90575 z + 7.9044 z^2 + 7.8061 z^3 + 0.37986 z^4}{1 - 0.98965 z + 7.9628 z^2 + 7.1435 z^3} \quad (5.8)$$

The approximants from the $g \neq 0$ analysis will be studied in the coming Section.

5.3. Scaling Function Case (ii)

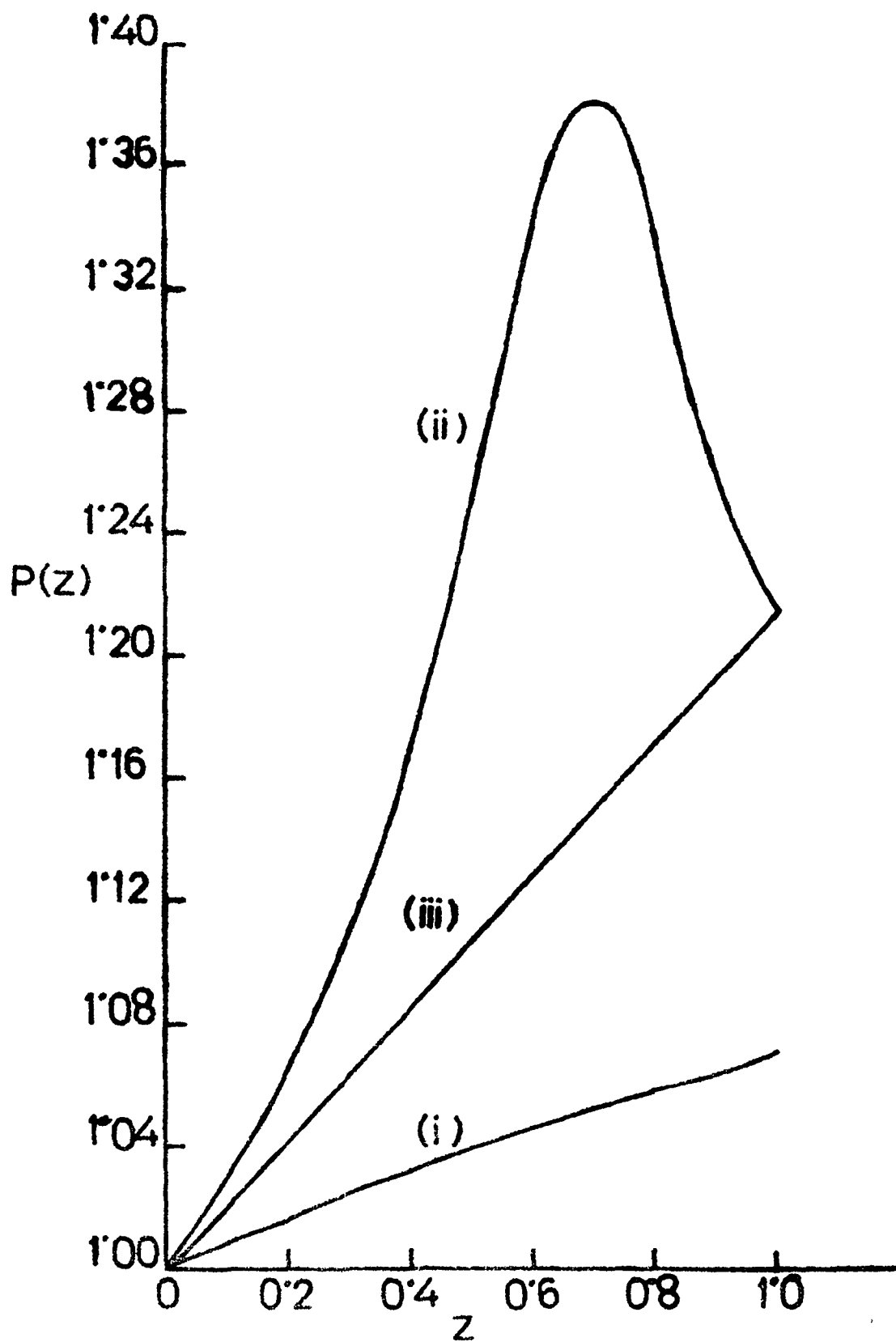
In the previous Section, we have shown how the isotropic scaling function for large x behaviour can be obtained and also how to interpolate between the small x and large x behaviour by obtaining approximants to $P(z)$ defined in equation (5.4) and using the conditions given in (5.7). In a similar fashion, we study the $g \neq 0$ scaling function in this Section.

For this case, the same set of P.A. taken in case (i)

Table 12. Coefficients of Padé Approximants for various $P(z)$ for $\bar{x} = 1.530$ and $\bar{x} = 1.216$.

Coefficients	(2,5)	(3,4)	(5,2)	(2,4)	(3,3)	(4,2)	(4,3)
P_0	1	1	1	1	1	1	1
P_1	21.9483	-1.0007	-6.1533	-1.2768	-1.2094	-1.4853	1.4008
P_2	.0386	-1.7373	6.0811	-0.10513	-0.50332	0.16514	-2.4628
P_3		2.4125	1.1607		0.58855	0.06930	2.1106
P_4			-0.04564			-0.12043	0.35301
P_5			0.69274				
q_0	1	1	1	1	1	1	1
q_1	21.6683	-1.280	-6.4333	-1.5568	-1.4894	-1.7653	-0.68088
q_2	-37.3052	-1.5782	7.6830	0.13132	-0.28573	0.45996	-2.4716
q_3	5.83101	2.8172		-0.01886	0.67302		2.6459
q_4	-0.83658	-0.40368		0.1302			
q_5	2.9893						

Fig. 8



are also calculated except that here $\dot{x} = 1.530$ and $\dot{X} = 1.216$. Their values are presented in Table 12. Again, by looking at the zeros and the poles of these approximants, we find that most of them are quite smooth and agree with one another upto 0.5%. For further work, we have chosen the $[3,4]$ approximant, which is

$$(ii) \quad P(z) = \frac{1 - 1.0007 z - 1.7373 z^2 + 2.4125 z^3}{1 - 1.2807 z - 1.5782 z^2 + 2.8172 z^3 + 0.40368 z^4} \quad (5.9)$$

In addition to the above two cases, we have also utilized the simplest form for $P(z)$, viz.,

$$(iii) \quad P(z) = 1 + (\dot{X} - 1) z \quad , \quad (5.10)$$

with

$$\dot{x} = 1.530 \quad , \quad \dot{X} = 1.216 \quad ,$$

in our analysis. For comparison, plots of these three selected values of $P(z)$ versus z are presented in Figure 8.

Now we comment on the behaviour of $P(z)$ versus z in the three cases. The case (ii) show a broad maximum. It is absent in case (iii) by construction, while in case (i) it is absent, we believe, due to the following reason. This approximant is obtained from the series $X(x)$ using the parameter $\dot{x} = 1.334$, which has been determined by direct analysis as the singular point of $X(x)$. Furthermore, the two-point Pade forces it to pass through $(z = 1, P(1) = \dot{X} = 1.071)$, the value of \dot{X} having estimated as the amplitude of $X(x)$ directly. In case (ii), however, $P(z)$ is required to pass through the point $(z = 1, P(1) = \dot{X} = 1.216)$ obtained along with $\dot{x} = 1.530$ from an entirely different ($g \neq 0$) analysis.

The next step in our analysis, is to study the cross-over behaviour of the exponent of the susceptibility $\chi(q, T)$. This will be discussed in the coming Section.

5.4. The Effective Exponent

So far we have obtained a representation of the scaling function for the diverging susceptibility, viz.,

$$\chi(q, T) \approx A \dot{t}^{-\gamma} \left[1 - \frac{x}{\dot{t}} \right]^{-\gamma} P(z) \quad (5.11)$$

where $z = x/\dot{t}$ and $x = Bg/\dot{t}^\phi$. The values of all the parameters involved in the above relation have been given in the previous Chapters. The set of universal constants x and \dot{t} and the corresponding universal functions $P(z)$ are given in equations (5.8), (5.9) and (5.10). It is to be noted that the representation (5.11) is valid only in the scaling regime, $g \ll 1$ and $\dot{t} \ll 1$.

An "effective exponent", γ_{eff} can be defined analytically through,^{45,88,89}

$$\gamma_{\text{eff}}(T, g) \equiv [T_c(g) - T] \left[\frac{\partial \ln \chi}{\partial T} \right]. \quad (5.12)$$

(Another equivalent approach is plotting $\ln \chi$ versus $\ln \dot{t}$, which may be closer to an experimental determination). Using equation (5.9), it is easily shown that in the scaling regime,

$$\gamma_{\text{eff}}(T, g) = \frac{\dot{t}}{t} \left(\gamma + \gamma \phi \frac{z}{1-z} + \phi z \frac{P'(z)}{P(z)} \right). \quad (5.13)$$

Now as $g \rightarrow 0$ at fixed temperature T , $\gamma_{\text{eff}}(T, g \rightarrow 0) \rightarrow \gamma$.

Fig. 9a

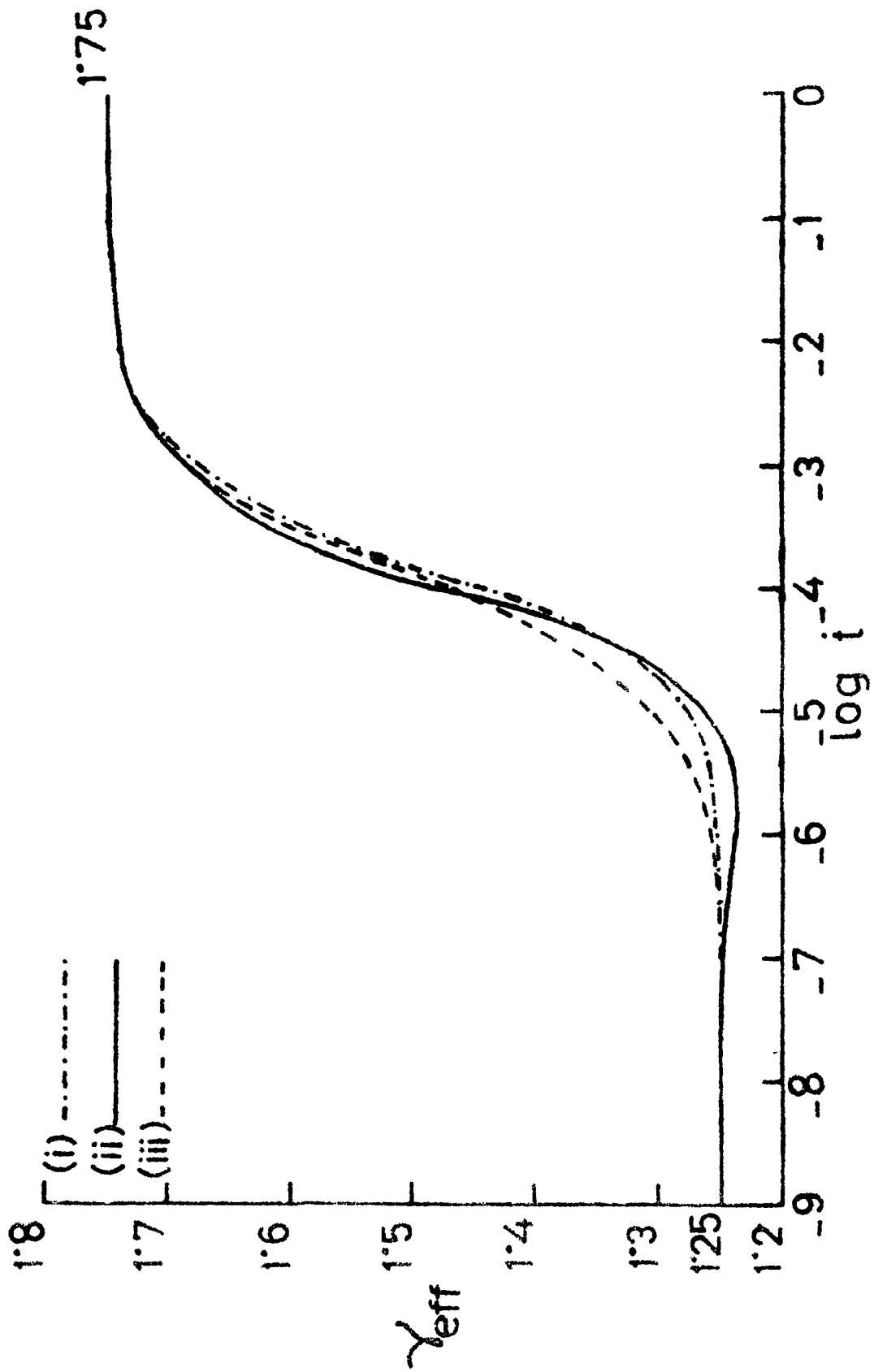


Fig. 9b

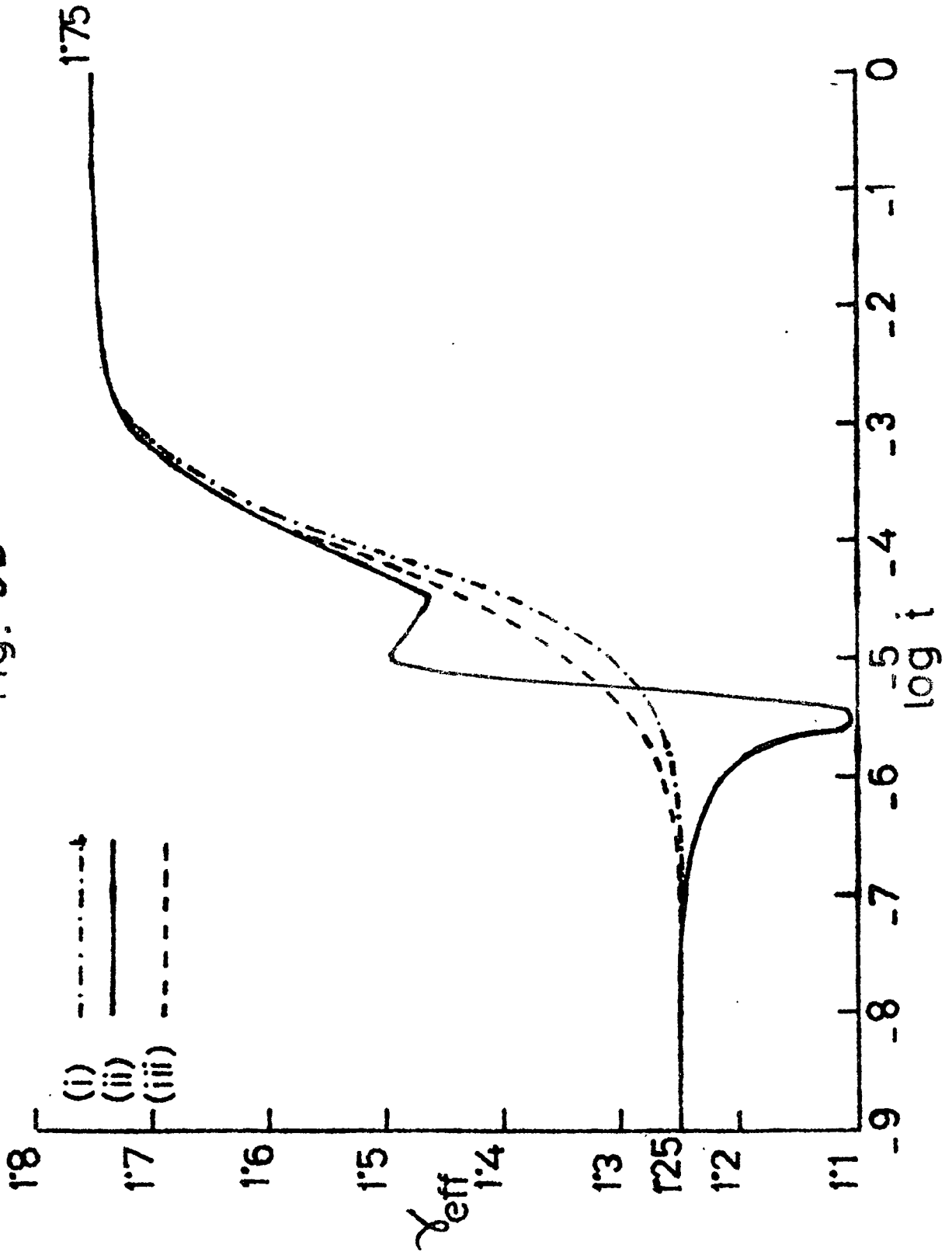


Fig. 10a

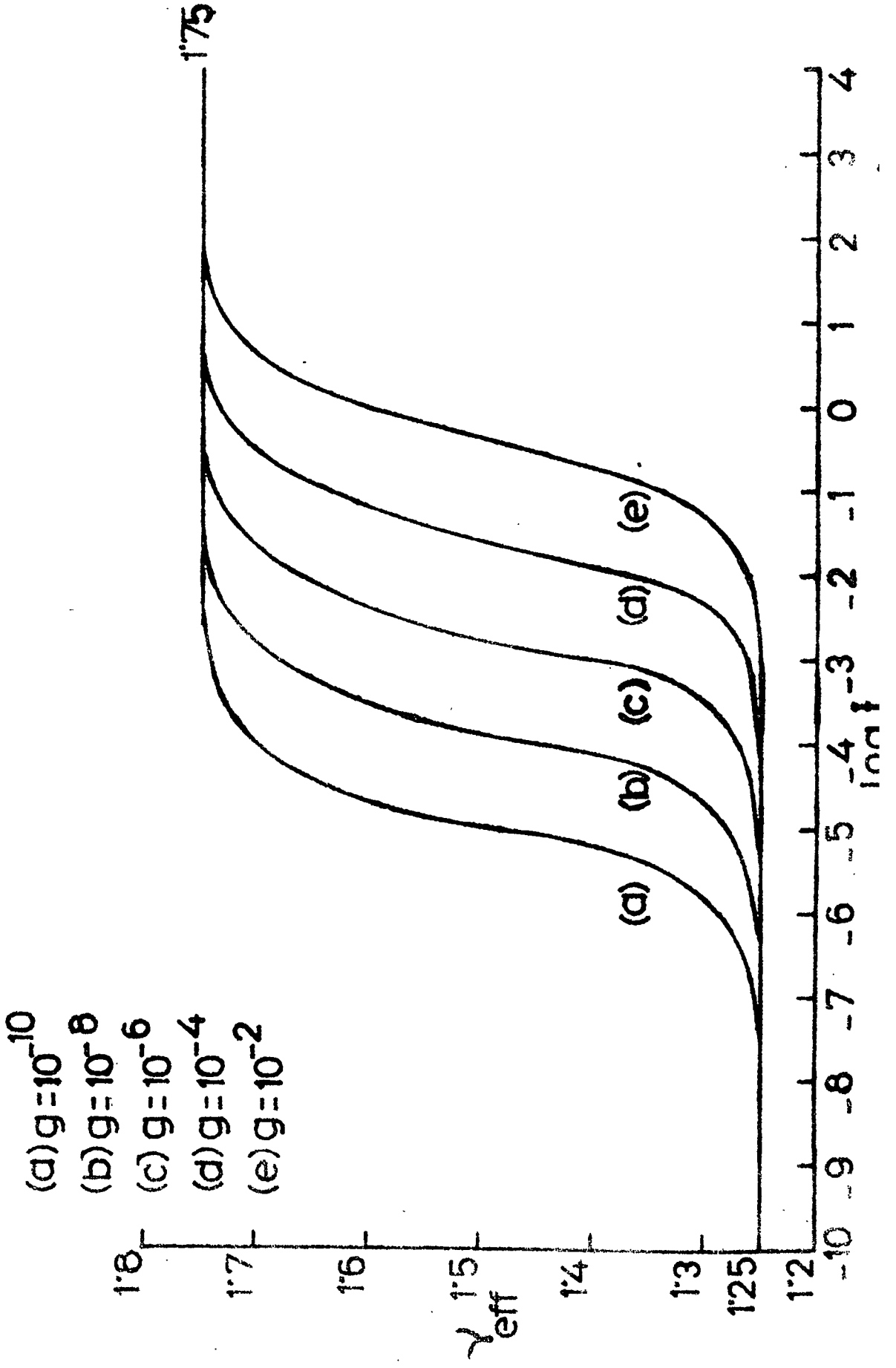
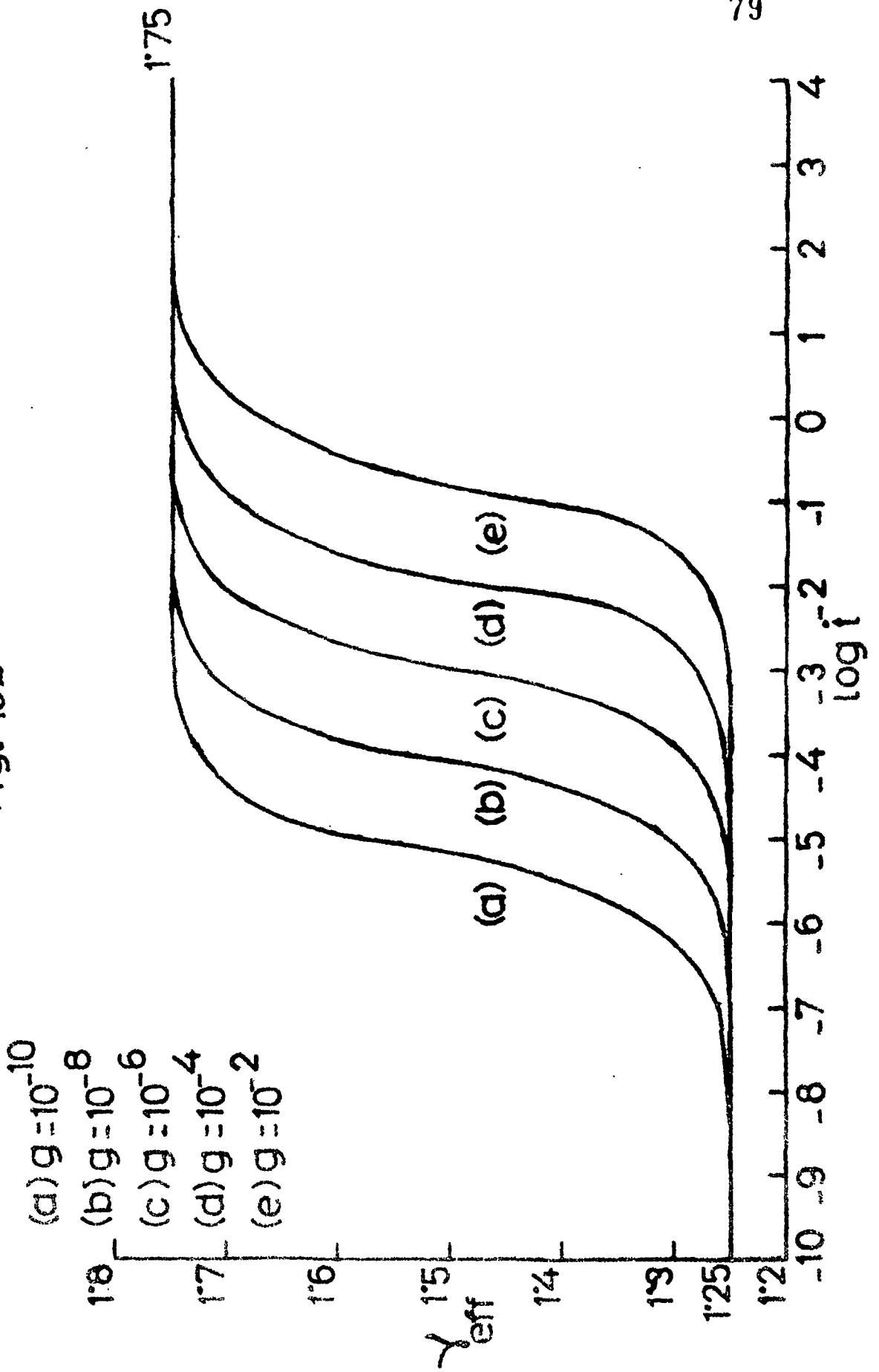


Fig. 10b



On the other hand, if g is fixed at a small, positive value and $T \rightarrow T_c(g)$, i.e., $t \rightarrow 0$, $\gamma_{\text{eff}}(T \rightarrow T_c(g), g) \rightarrow \gamma$, as expected. The detailed behaviour between these two limits will depend on the non-universal parameters relating to the lattice type and model, and also on the choice of $P(z)$. Since we have obtained all the relevant parameters in the preceding Sections we can now calculate γ_{eff} using (5.13). Figures 9 a,b display the plots of γ_{eff} versus $\log t$ for $g = 10^{-8}$. Curves (i), (ii) and (iii) correspond to the three choices of $P(z)$ (see equations 5.8, 5.9 and 5.10). Curves (i) and (iii) are smooth but the curves (ii) show some structure mainly in the region where the anisotropic effects predominate. Therefore, we concentrate mainly on the choice (i) because it gives smooth γ_{eff} and utilizes the full series (3.35). In Figures 10a,b we show the graphs of γ_{eff} against $\log t$ for various values of g . Since the critical region is usually for $t \leq 10^{-2}$, one should not take the graphs seriously beyond this reduced temperature. Also for $t \geq 10^{-2}$ there is expected to be a crossover to the mean-field exponent of unity.

From Figures 10a,b it can be seen that the effective exponent will start to deviate from $\gamma = 1.75$ near $t \approx 10^{-2}$. These curves show the crossover of $\gamma_{\text{eff}}(T, g)$ from γ to γ for fixed values of g . All the curves start from $\gamma = 1.25$, rise smoothly and go to $\gamma = 1.75$, as t increases. For $g \leq 10^{-8}$, our graphs predict a gradual crossover from 1.75 to 1.25 as one goes towards the critical temperature. For $g \geq 10^{-8}$, one may not see a complete crossover to the isotropic value of 1.75. Thus, experiments in the range $g \gtrsim 10^{-8}$ and $t \lesssim 10^{-2}$ may yield intermediate values of γ . Finally, it should be noted that the crossover region is about four decades in t for a given value of g . Its width is practically independent of lattice type as it depends mainly on the crossover exponent. In using the crossover analysis one must remember that it is not

designed to describe the behaviour outside the critical region; alternative analyses exist to describe the behaviour over the full high-temperature region, see for example Reference 66.

This completes our study of the crossover behaviour of the susceptibility $\chi(q, T)$ of the quasi-two-dimensional Ising model.

Table 13. Values of Non-Universal Parameters for various Two- to Three-dimensional Crossovers.

Parameter	s.o. to s.c.	s.o. to f.o.c.	s.o. to b.o.c.	p.t. to f.o.c.
$K_c(0)$	0.44068679	0.44068679	0.44068679	0.27465307
A	0.96258173	0.96258173	0.96258173	0.92420696
λ	2	8	4	6
B	0.84839414	3.3935766	1.6907883	1.5230177
μ	0.7139	1.5765	1.0610	0.9974
Λ_∞	0.6882	0.4632	0.5646	0.5591

General Remarks and Conclusions

6.1. General Remarks : Other Lattices and Related Models

We have studied the lattice-anisotropy crossover for the s.q. to s.c. and s.q. to f.c.c. lattices only. However, following modern ideas about universality, we expect the scaling function $X(x)$ to be universal for all other crossovers from two to three dimensions. Only the values of the non-universal parameters will depend on the lattice type.

Since all the two-dimensional lattices with nearest neighbour interactions have been solved exactly, the values of A and $K_c(0)$ are known.^{14,45} The value of B follows from Liu-Stanley relations⁷⁴

$$\left(\frac{\partial \chi}{\partial g}\right)_0 = \lambda K [\chi(0)]^2,$$

where λ is the number of extra interactions in the off-plane directions. Then from the universal values of x and X one can get the values of ω and A_∞ . For illustration, we display the results for s.q. to b.c.c. and triangular to f.c.c. crossovers in Table 13. (For completeness, we also collect the results for

the s.q. to s.c. and s.q. to f.c.c.). Other lattices can be dealt with similarly.

As examples of related models, consider our Hamiltonian (equation 1.8), in the s.c. case. We have considered the case (i) $J > 0$, $g > 0$. For the other choices of signs, we have the following three possibilities:

- (ii) $J > 0$, $g < 0$,
- (iii) $J < 0$, $g > 0$,
- (iv) $J < 0$, $g < 0$.

All these cases can be studied by making appropriate scaling hypotheses in a manner similar to our case. The only difference is that the usual susceptibility will not be the ordering susceptibility in these cases. In case (ii), χ will diverge strongly for $g = 0$ but only weakly for $g \neq 0$. In cases (iii) and (iv), even the $g = 0$ susceptibility will diverge only weakly. All these cases can be handled by using the techniques of Gerber and Fisher⁹⁰ who discussed a similar problem for the case of spin-space anisotropy.

6.2. Comparison of our Results with others

Even though our results verify the scaling and universality theories and are internally consistent, it would be very useful to study the model by using other methods. We have already compared our results of $\dot{\omega}$ and A_{∞} with those of Harbus and Stanley^{76b} in Section 4.3.

The problem of obtaining the scaling function can be attacked by renormalization group (RG) technique, newer extrapolation methods and experiments.

There has been considerable interest recently in the RG approach to the theory of critical phenomena.^{40,41} For our model, Grover⁷⁸ and Chang and Stanley⁷⁹ proved that $\phi = \gamma$ using these methods. Bruce⁸⁰ studied the problem of obtaining the scaling function. But so far, the scaling function has not been obtained by these methods. Therefore, it would be highly desirable if the scaling function can be obtained using the RG method, which will be an indirect check on our calculations.

Recently, a more powerful technique, the partial differential approximants technique⁹¹ for the series analysis has been developed. An application of this method to several test functions and dimensional crossover in the Ising model was made by Stilck and Salinas.⁹² Again, there have not been a calculation of the crossover scaling function by this method. It would be of great interest to apply this method to the present problem.

Regarding experimental studies,⁶⁷ there are very few of them but in most cases, either one or both of the interactions J and J' are antiferromagnetic. The only known example⁶⁷ of the present model is perhaps FeCl_2 . In this case, the value of g is estimated to be 7.5×10^{-2} , but from our study of the effective exponent, we can easily see that this value of g is outside the crossover scaling region.

Thus, further work, both experimental and theoretical, would be most welcome.

6.3. Concluding Remarks

We have studied the crossover behaviour of the susceptibility of quasi-two-dimensional Ising models, occurring when small anisotropic exchange interactions are introduced into an otherwise isotropically coupled system. The two lattices studied are s.c. and f.c.c. lattices. It has been shown, with good numerical precision, that a scaling formulation describes the crossover of the susceptibility. We have verified the detailed predictions of the extended crossover scaling theory both for $g = 0$ and $g \neq 0$ and have obtained accurate estimates for the non-universal and universal parameters.

By studying derivatives of the susceptibility with respect to the anisotropy in the isotropic limit, we have obtained the expansion for the scaling function $X(x)$, in powers of x . Furthermore, the universality of the expansion with respect to lattice structure has been convincingly demonstrated for the two lattices studied.

In addition, we have done careful analyses for finite, non-vanishing values of anisotropy to reveal the universality of the scaling function $X(x)$, in particular, to evaluate the singular behaviour as x approaches a characteristic critical value x related directly to the anisotropy-induced shift in critical temperature. In this way, we have been able to construct accurate approximants to a crossover scaling function valid in the whole critical region.

The crossover of the effective susceptibility exponent, γ_{eff} , has been studied over a wide range of temperatures for a range of anisotropies. The results indicate that the full

crossover behaviour may be experimentally unobservable for physical anisotropies of a few percent.

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1. Thermal and Magnetic Properties of Quasi-one-dimensional Magnetic Systems, Nucl. Phys. and Solid State Physics 23C, in print (1980).
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All these papers are with Dr. Surjit Singh.

