

Crossover scaling function for the lattice anisotropy of the quasi-two-dimensional Ising models: the susceptibility

W L Basaiawmoit and Surjit Singh

Department of Physics, North-Eastern Hill University, Shillong-793003, India

Received 9 June 1982

Abstract. The crossover scaling behaviour for the lattice anisotropy of the susceptibility of the quasi-two-dimensional Ising models has been studied using high-temperature series expansions. The predictions of the extended scaling hypothesis are verified and the plots of the effective exponent are presented in the scaling regime. These results should provide a basis for comparison with experiments on quasi-two-dimensional Ising systems.

1. Introduction

Quasi-two-dimensional systems, i.e., three-dimensional systems in which interactions in the off-plane directions are weaker than those within the planes, have been of recent experimental interest (see the recent reviews by De Jongh and Miedema 1974, De Jongh and Stanley 1976, De Jongh 1976). The most important parameter determining the behaviour of such a system is the lattice anisotropy g , i.e., the ratio of the off-plane to intraplanar couplings. For g large, say more than about 10^{-2} , the properties of the system are essentially three-dimensional in nature. So one can use the standard Padé approximant methods to construct the thermodynamic functions for all temperatures. This was recently done by Navarro and De Jongh (1978). On the other hand, for smaller values of g , the behaviour of the system is two-dimensional for temperatures not too close to the critical temperature $T_c(g)$ and crosses over to the true three-dimensional behaviour only when $T_c(g)$ is approached more closely. In this case, the behaviour is nicely described by a crossover scaling hypothesis introduced by Riedel and Wegner (1969). The thermodynamic functions showing this subtle behaviour can now be obtained by using the methods developed in the analogous case of spin-space anisotropy by Pfeuty *et al* (1974; hereafter PJF). Experimentally, the results for both the susceptibility and the specific heat are generally available, but, the former (because of its stronger singularity) is more suitable for an initial study of the critical behaviour. In this paper, we concentrate on the crossover scaling functions and approximants for the susceptibility; in a later publication, we plan to report on specific heat and comparison with experiments (W L Basaiawmoit and S Singh, work in progress).

The outline of this paper is as follows. In § 2, we give a brief summary of the scaling theory and the previous work. The detailed isotropic ($g = 0$) and the anisotropic behaviours are given in §§ 3 and 4. The scaling functions are obtained and the plots for effective exponents are given in § 5. Our concluding remarks are in § 6.

2. The scaling theory and the previous work

We shall be dealing with the ferromagnetic quasi-two-dimensional Ising model Hamiltonian

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

where the first summation is over all the NN pairs of spins within the planes parallel to the xy plane and the second summation is over all other NN pairs. For $g = 0$, the Hamiltonian (1) describes a set of mutually non-interacting two-dimensional Ising models. In this case, the zero-field reduced susceptibility is given by

$$\chi(g = 0, T) \approx A t^{-\gamma} \quad t = [T - T_c(0)]/T_c(0) \quad (2)$$

in the critical region. (For definitions of exponents etc, see the review by Fisher (1967) and the monograph by Stanley (1971).) For $g \neq 0$, the critical temperature shifts to $T_c(g)$ and it is convenient to introduce

$$t = [T - T_c(g)]/T_c(0).$$

The general scaling theory (Riedel and Wegner 1969) implies for the susceptibility that

$$\chi(g, T) \approx A t^{-\gamma} \tilde{X}(\tilde{B}g/t^\varphi),$$

for $g, t \rightarrow 0$, where φ is the crossover exponent. This leaves open the question of the shift exponent defined through

$$t_c(g) \equiv [T_c(g) - T_c(0)]/T_c(0) \approx \psi g^{1/\psi} \quad g \rightarrow 0. \quad (3)$$

However, generally, $\psi = \varphi$ (see Singh (1975) for many examples of this in the spherical model). In that case the theory implies further that

$$\chi(g, T) \approx A t^{-\gamma} X(Bg/t^\varphi) \quad (4)$$

(M E Fisher and D Jasnow, unpublished; PJF. We shall exclusively use this extended version of the theory).

Now, we summarise the detailed predictions of the theory following PJF. The successive derivatives of χ at $g = 0$ should diverge as,

$$\Xi_m \equiv (\partial^m \chi / \partial g^m)_0 \approx C_m t^{-(\gamma - m\varphi)} \quad t \rightarrow 0. \quad (5)$$

With the normalisations,

$$X(0) = 1 \quad (dX/dx)_0 = 1 \quad (6)$$

we see that

$$C_0 = A \quad C_1 = AB \quad (7)$$

and

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

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

$$X(x) \approx \dot{X}(1 - x/\dot{x})^{-\dot{\gamma}} \quad x \rightarrow \dot{x}. \quad (8)$$

This results in the following predictions. The quantity \dot{x} is universal and is given by

$$\dot{x} = B\dot{w}^{-\varphi}. \quad (9)$$

The amplitudes $\dot{A}(g)$ in the $g \neq 0$ behaviour of χ i.e.,

$$\chi(g, T) \approx \dot{A}(g)i^{-\dot{\gamma}} \quad i \rightarrow 0 \quad (10)$$

diverge as

$$\dot{A}(g) = A_\infty g^{(\dot{\gamma}-\gamma)/\varphi} \quad g \rightarrow 0, \quad (11)$$

with the universal amplitude \dot{X} given by

$$\dot{X} = A_\infty \varphi \dot{w}^{\dot{\gamma}-\gamma}/A. \quad (12)$$

(The so-called double power law behaviour of the amplitude in (11) also follows from the original Riedel–Wegner theory.) After this brief summary of the scaling theory, we summarise previous work.

This model has been studied extensively; for recent reviews, see Domb (1974) and Stanley (1974). After some initial controversy (Oitmaa and Enting 1971, 1972, Rapaport 1971, Paul and Stanley 1971, Enting and Oitmaa 1971) and some heuristic arguments (Abe 1970, Suzuki 1971, Coniglio 1972), Liu and Stanley (1972, 1973) and Citeur and Kasteleyn (1972) showed rigorously that

$$\varphi = \gamma. \quad (13)$$

Subsequently, Harbus and Stanley (1973a, b) and Krasnow *et al* (1973) analysed the high-temperature series for the anisotropic sc and FCC lattices and produced strong support for (13). Estimates for critical temperatures and amplitudes were obtained by Harbus and Stanley (1973b) who tested the relations (3) and (11) by Padé approximant methods. They found that the simple power law relations are valid with the expected exponents. In the meantime PJF and Singh and Jasnow (1975) developed and applied suitable methods for calculating the scaling functions for the analogous case of the spin-space anisotropy. In this paper, we have essentially used these methods for the study of lattice-space anisotropy. We present the details of our analysis in the coming sections. (Brief, preliminary accounts of this work have been reported earlier; Basaiawmoit and Singh (1982a, b).)

3. Isotropic ($g = 0$) critical behaviour

In this section, we obtain the $g = 0$ behaviour of the Hamiltonian (1). We will deal with

the cases SQ to SC and SQ to FCC. For $g = 0$, we get a set of SQ Ising models. The critical temperature of this model is exactly known to be given by

$$K_c(0) = J/k_B T_c(0) = \frac{1}{2} \ln(1 + \sqrt{2}) = 0.440686793 \dots \tag{14}$$

(Kramers and Wannier 1941, Onsager 1944). The susceptibility exponent γ is equal to 1.75 (This has a long history; see the review by Domb 1974). So from (13), it follows that $\varphi = 1.75$. The latest estimate for the critical amplitude A in (2) was given by Sykes *et al* (1972); the exact value was obtained by Barouch *et al* (1973). They calculated that

$$A(\text{SQ}) = 0.9625817322 \dots \tag{15}$$

in complete agreement with the former authors. (We may remark in passing that these authors also found confluent singularities in the asymptotic behaviour of the susceptibility. 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 g . So, we have concentrated only on the leading crossover behaviour for small g .) Once the value of A is known, that of B follows from the work of Liu and Stanley (1972, 1973) who proved many rigorous thermodynamic relations, in particular,

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

where λ denotes the number of *extra* interactions in the off-plane directions. It is equal to 2 and 8, respectively, for the cases of SC and FCC lattices. This helps us to get B exactly; we obtain,

$$B(\text{SQ to SC}) = 0.848394142 \dots \tag{16a}$$

$$B(\text{SQ to FCC}) = 3.39357656 \dots \tag{16b}$$

Equations (7), (15) and (16) give us C_0 and C_1 exactly. To get the other values of C_m , high-temperature series analysis is resorted to. The series for the susceptibility for the cases SQ to SC (to 11th order) and SQ to FCC (to 10th order) in powers of $\tanh K$ are given in Oitmaa and Enting (1971), and Harbus and Stanley (1973a), respectively. For convenience, we have converted the series to the form,

$$\begin{aligned} \chi(g, K) &= \sum_{n=0}^{\infty} a_n(g) K^n \\ a_n(g) &= \sum_{l=0}^n b_n g^l \end{aligned} \tag{17}$$

The coefficients b_{nl} , so obtained, are given in table 1 for the FCC lattice. Knowing the exact values of $K_c(0)$, γ and φ , we have calculated the series for

$$C_m(K) = [1 - K/K_c(0)]^{\gamma + m\varphi} \Xi_m$$

and then used the standard ratio and Padé methods to estimate the critical amplitudes. We have also performed the ratio and the Padé analyses for the series for

$$R_m(K) = \frac{\Xi_{m-1} \Xi_{m+1}}{\Xi_m^2} \tag{18}$$

(For a recent review of these methods, see Gaunt and Guttman 1974). As an example, Padé approximants to the SC series for $R_m(K)$ for $m = 1-5$ evaluated at $K = K_c(0)$ are shown in table 2. On the whole, we find that the standard methods give consistent results

except for the PAS to the $R_m(K)$ series for the FCC 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, along with the mean-field results and universal values adopted for further work are listed in table 3. Our confidence limits based on overall analysis are 1, 1, 2, 3 and 5% in the amplitudes R_1-R_5 , respectively.

Table 1. Reduced susceptibility expansion coefficients b_{nl} , defined in (17) for the sq to FCC case.

n	l	b_{nl}	n	l	b_{nl}
0	0	1	7	5	4993002 $\frac{2}{3}$
1	0	4	7	6	3053159 $\frac{4}{3}$
1	1	8	7	7	759545 $\frac{4}{3}$
2	0	12	8	0	3809 $\frac{87}{105}$
2	1	64	8	1	160939 $\frac{11}{3}$
2	2	56	8	2	1811017 $\frac{4}{3}$
3	0	34 $\frac{2}{3}$	8	3	9584969 $\frac{4}{3}$
3	1	320	8	4	27327480 $\frac{8}{3}$
3	2	656	8	5	45609776 $\frac{4}{3}$
3	3	389 $\frac{1}{3}$	8	6	43961545 $\frac{4}{3}$
4	0	92	8	7	22924237 $\frac{8}{3}$
4	1	1322 $\frac{2}{3}$	8	8	4966694 $\frac{11}{3}$
4	2	4544	9	0	9364 $\frac{11888}{315}$
4	3	5994 $\frac{2}{3}$	9	1	477876 $\frac{88}{315}$
4	4	2610 $\frac{2}{3}$	9	2	6561420 $\frac{11}{3}$
5	0	240 $\frac{8}{15}$	9	3	42946637 $\frac{104}{15}$
5	1	4842 $\frac{2}{3}$	9	4	154892344 $\frac{8}{3}$
5	2	24501 $\frac{1}{3}$	9	5	339157477 $\frac{4}{3}$
5	3	52789 $\frac{1}{3}$	9	6	456207197 $\frac{88}{315}$
5	4	49866 $\frac{2}{3}$	9	7	372564564 $\frac{11}{3}$
5	5	17473 $\frac{1}{15}$	9	8	168266475 $\frac{4}{3}$
6	0	611 $\frac{1}{3}$	9	9	32458605 $\frac{8811}{315}$
6	1	16392 $\frac{8}{15}$	10	0	22820 $\frac{4428}{315}$
6	2	113258 $\frac{2}{3}$	10	1	1382060 $\frac{188}{315}$
6	3	350577 $\frac{2}{3}$	10	2	22672635 $\frac{71}{315}$
6	4	532538 $\frac{2}{3}$	10	3	179063707 $\frac{11}{3}$
6	5	398216 $\frac{8}{15}$	10	4	791598100 $\frac{37}{315}$
6	6	115250 $\frac{22}{3}$	10	5	2176311440 $\frac{18}{315}$
7	0	1538 $\frac{88}{315}$	10	6	3818160361 $\frac{87}{315}$
7	1	52451 $\frac{1}{3}$	10	7	4327624997 $\frac{37}{135}$
7	2	470871 $\frac{7}{15}$	10	8	3046735819 $\frac{71}{315}$
7	3	1950289 $\frac{2}{3}$	10	9	1219450540 $\frac{8211}{315}$
7	4	4202769 $\frac{2}{3}$	10	10	211100973 $\frac{11384}{153075}$

It is seen from table 3, that the central estimates for the ratios R_m agree with each other very well. This implies that the prediction of the scaling theory about the universality of these ratios is very well fulfilled. We test the predictions of the theory about the $g \neq 0$ behaviour in the next section.

Table 2. Padé estimates for the universal ratios for the sc lattice. The numbers are the values of the PAS to the series (18) at $K = K_c(0)$. The symbol—means a defective entry, NC means not calculated.

Padé	R_1	R_2	R_3	R_4	R_5
(1, 1)	NC	NC	NC	1.3781	1.3369
(1, 2)	NC	NC	NC	—	0.2264
(2, 1)	NC	NC	NC	—	—
(2, 2)	1.7918	1.4862	1.2617	1.1791	1.1238
(2, 3)	1.0650	1.4617	1.4483	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 3. Overall estimates for the universal amplitude ratios R_m . For confidence limits, see text.

Ratio	FCC	SC	Adopted mean	Mean-field value
R_1	1.6703	1.6715	1.6709	2
R_2	1.4793	1.4718	1.4755	1.5
R_3	1.2914	1.2924	1.2919	1.333 . . .
R_4	1.2599	1.2410	1.2505	1.25
R_5	1.1243	1.1402	1.1323	1.2

4. Anisotropic critical behaviour

The scaling theory makes definite predictions (mentioned in § 2) about the small- g behaviour. However, for very small values of g , one needs correspondingly very long series for a reliable analysis. On the other hand, the scaling theory does not apply for large enough g . So, for the crossover scaling analysis, there is a typical ‘window’ of values of g . An estimate of this range can be obtained by making a scaling hypothesis for the coefficients $a_n(g)$ themselves (see PJF);

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

$$F(0) = 1.$$

This predicts, e.g., that the sequence

$$\dot{w}_n = g^{-1/\nu} \left(\frac{n\rho_n(g)K_c(0)}{n + \gamma - 1} - 1 \right)$$

where,

$$\rho_n(g) = a_n(g)/a_{n-1}(g)$$

should vary as

$$\dot{w}_n \approx \dot{w} + (\dot{\gamma} - \gamma)/ng^{1/\varphi} \quad ng^{1/\varphi} \rightarrow \infty.$$

On applying this method to our case, we find that ranges of g amenable to analysis are $0.01 \leq g \leq 0.08$ and $0.005 \leq g \leq 0.02$ for the SC and the FCC cases, respectively. This is in general agreement with the previous work of Harbus and Stanley (1973b), who obtained similar ranges by a different method.

Having decided on a range of values of g to work with, the next step is to estimate the critical temperatures. Here, apart from the standard methods (Gaunt and Guttman 1974), PJF extrapolated the sequences,

$$\mu_n(g) = \left(\frac{n + \delta}{n + \delta + \dot{\gamma} - \gamma} \right) \frac{\rho_n(g)}{\rho_n(0)}, \tag{19}$$

versus n^{-2} . In our work, we have used these as well as the standard techniques. It is found that in both the cases under study, the method using the extrapolants (19) works well; whereas the conventional methods, e.g., using

$$\tilde{\mu}_n(g) = \frac{(n + \delta) \rho_n(g)}{(n + \delta + \dot{\gamma} - 1)}$$

show oscillations due to the loose-packed nature of the SQ lattice. In $\mu_n(g)$, these oscillations are cancelled to a large extent because the ratio $\rho_n(g)/\rho_n(0)$ is used. The graphs of $\mu_n(g)$ against n^{-2} for several values of g are shown in figure 1. These methods

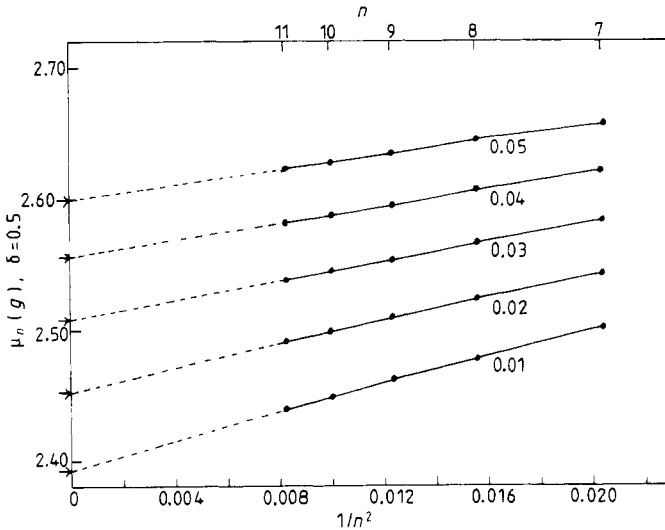


Figure 1. The graphs of sequences $\mu_n(g)$ (see equation (19)) against n^{-2} for $g = 0.01$ to 0.05 for the SC lattice. The arrows point to the chosen values of $[K_c(g)]^{-1}$. Values of g are given on curves.

allow us to estimate the critical temperatures to an accuracy of about a conservative 0.2%. This uses the exact values of γ , $K_c(0)$ and also assumes that the three-dimensional exponent $\dot{\gamma}$ is *exactly* 1.25 (Domb 1974). Our estimates of $K_c(g)$ are listed in table 4. Now we calculate

$$\dot{w}_{\text{eff}}(g) = [K_c(0) - K_c(g)]/[K_c(0)g^{1/\varphi}].$$

Table 4. Estimates of critical temperatures $K_c(g) = J/k_B T_c(g)$ and amplitudes $\dot{A}(g)$ for various values of the anisotropy parameter g . The critical temperatures are believed to be accurate to about 0.2% and the amplitudes to about 4%.

FCC			SC		
g	$K_c(g)$	$\dot{A}(g)$	g	$K_c(g)$	$\dot{A}(g)$
0.006	0.40355	1.985	0.01	0.41806	2.495
0.008	0.39730	1.861	0.02	0.40766	2.135
0.010	0.39093	1.706	0.03	0.39872	1.878
0.012	0.38595	1.647	0.04	0.39124	1.722
0.014	0.38110	1.5755	0.05	0.38476	1.624
0.016	0.37636	1.505	0.06	0.37893	1.543
0.018	0.37202	1.4535	0.07	0.37341	1.469
0.020	0.36792	1.4055	0.08	0.36846	1.4175

(Here we have accepted $\psi = \varphi$; plotting $\log[K_c(0) - K_c(g)]$ against $\log g$ confirms this, see also Harbus and Stanley 1973b). Extrapolation of $\dot{w}_{\text{eff}}(g)$ to $g = 0$ with g or $g^{1/\varphi}$ yields the estimates,

$$\dot{w} = 0.715 \pm 0.025 \text{ (SC)} \quad (20a)$$

$$\dot{w} = 1.575 \pm 0.055 \text{ (FCC)}. \quad (20b)$$

The uncertainties in \dot{w} reflect mainly those in $K_c(g)$. Clearly, these critical point shift amplitudes are non-universal. On using (9), (16) and (20), we calculate \dot{x} to get,

$$\dot{x} = 1.526 \pm 0.090 \text{ (SC)} \quad (21a)$$

$$\dot{x} = 1.533 \pm 0.090 \text{ (FCC)}. \quad (21b)$$

It is seen that the central estimates agree with each other to about $\frac{1}{2}\%$; the scale factor universality is very well satisfied.

Now we are in a position to evaluate the critical amplitudes $\dot{A}(g)$ in (10). We use conventional ratio methods based on the extrapolation of

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

against n^{-1} which are found to work well in both the cases (SC and FCC). Our estimates are listed in table 4. Uncertainties in the amplitudes are about 4% and come mainly from those in $K_c(g)$. Now we form

$$(A_\infty)_{\text{eff}} = \dot{A}(g) g^{(\gamma - \dot{\gamma})/\varphi}$$

which are found to have a weak dependence on g ; they are extrapolated against g or $g^{1/\varphi}$ to give

$$A_\infty = 0.690 \pm 0.040 \quad \text{(SC)} \quad (22a)$$

$$A_\infty = 0.462 \pm 0.025 \quad \text{(FCC)}. \quad (22b)$$

From these estimates, we form X , using (12), (15), (20) and (22). We get

$$\dot{X} = 1.220 \pm 0.070 \text{ (sc)} \quad (23a)$$

$$\dot{X} = 1.212 \pm 0.070 \text{ (FCC)}. \quad (23b)$$

Again, we see that the universality is satisfied to a good degree of accuracy.

For further work, we adopt the following 'best' values for the two universal parameters,

$$\dot{x} = 1.530 \quad \dot{X} = 1.216. \quad (24)$$

It is to be noted that we have mostly not used the Padé method in $g \neq 0$ analysis as that was already used by Harbus and Stanley (1973b) in their study of this model. Their aim was mainly to test the power law predictions (3) and (11). However, on using their figures (2a) and (3), we estimate the values of \dot{w} (A_∞) from their analysis to be consistently higher (lower) than our central estimates for the two models but within our confidence limits. With this, we have completed our analysis of the detailed predictions of the scaling theory both for $g = 0$ and $g \neq 0$. In the next section, we will construct approximants for the scaling functions using these results.

5. Scaling functions for lattice anisotropy

Having obtained detailed information about the scaling function $X(x)$ near $x = 0$ and $x = \dot{x}$, we now construct approximants for it. Using the adopted universal values of the ratios R_m , $m = 1-5$, we can form the low x expansion of $X(x)$ from

$$X(x) = 1 + x + \frac{1}{2!} R_1 x^2 + \frac{1}{3!} R_2^2 R_2 x^3 + \dots \quad (25)$$

(PJF and Liu and Stanley 1972). We get

$$X(x) = 1 + x + 0.83545 x^2 + 0.6866 x^3 + 0.5467 x^4 + 0.4355 x^5 + 0.3273 x^6 \dots \quad (26)$$

We emphasise again that we have verified that this scaling function is universal and following current ideas about universality, we expect it to be the same for *all* two- to three-dimensional crossovers in the Ising model (i.e. universal with respect to spin values, range of interactions as long as they remain short-ranged, lattice-type, etc.) The above representation of $X(x)$ is valid for $x \ll 1$; to extend its range to \dot{x} , we have to take into account its singularity at \dot{x} i.e. (8). Although the values of \dot{x} and \dot{X} have been obtained in § 4, it is useful to get estimates from the six-term series (26) itself, e.g., by forming Padé approximants to $[X(x)]^{1/\dot{X}}$. We get

$$\dot{x} = 1.334 \quad \dot{X} = 1.071. \quad (27)$$

(The relatively large differences between (24) and (27) are probably due to the shortness of the series (26), see PJF and Singh and Jasnow (1975).) Approximants for $X(x)$ valid up to \dot{x} may now be obtained by forming Padé approximants to the six-term series,

$$P(z) = (1 - z)^{\dot{X}} X(x) \quad z = x/\dot{x}$$

subject to the conditions

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

For the assignment (27), we have examined the (2, 4), (4, 2), (3, 3), (3, 4) and (4, 3) approximants. All of these are quite smooth for $0 \leq z \leq 1$ and agree with one another within less than $\frac{1}{2}\%$. We choose, somewhat arbitrarily, the following for future work:

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

$$\dot{x} = 1.334 \quad \dot{X} = 1.071. \tag{28}$$

We have examined the same set of PAs for the assignment (24). In this case, all 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 \dot{x} , so $P(z)$ should be smooth. So, we reject all PAs except (3, 4) and (4, 3) as unsuitable. These two PAs show a broad maximum at about $z = 0.7$ and agree with each other within 1%. A similar maximum was found in the case of spin-space anisotropy (PJF, Singh and Jasnow 1975). We choose the (3, 4) approximant:

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

$$\dot{x} = 1.530 \quad \dot{X} = 1.216. \tag{29}$$

In addition to (28) and (29), we have also utilised the simplest form for $P(z)$, i.e.

$$(iii) \quad P(z) = 1 + 0.216z$$

$$\dot{x} = 1.530 \quad \dot{X} = 1.216 \tag{30}$$

in our analysis.

To study the crossover behaviour of χ , we define an effective exponent through

$$\gamma_{\text{eff}}(g, T) = [T_c(g) - T] \left(\frac{\partial \ln \chi}{\partial T} \right) \tag{31}$$

(Kouvel and Fisher 1964, Riedel and Wegner 1974). Using the expression for χ in the form

$$\chi(g, T) \approx At^{-\gamma} \left(1 - \frac{x}{\dot{x}} \right)^{-\dot{\gamma}} P(z) \tag{32}$$

equation (31) can be simplified to give

$$\gamma_{\text{eff}}(g, T) = \frac{\dot{t}}{t} \left[\gamma + \dot{\gamma} \varphi \frac{z}{1-z} + \varphi \frac{zP'(z)}{P(z)} \right]. \tag{33}$$

This expression holds in the scaling region. For $g \rightarrow 0$ at fixed temperature, $\gamma_{\text{eff}} \rightarrow \gamma$ and for $g \neq 0, \dot{t} \rightarrow 0, \gamma_{\text{eff}} \rightarrow \dot{\gamma}$, as expected. The detailed behaviour between these two limits depends on the non-universal parameters of a given model. Since we have obtained all the relevant parameters in the preceding sections, we can calculate γ_{eff} from (33). In figures 2 and 3, we show the plots for $g = 10^{-8}$ for the SC and FCC lattices, respectively. Curves (i), (ii) and (iii) correspond to the choices for $P(z)$, equations (28) to (30). Curves (i) and (iii) are smooth but the curve (ii) shows some structure mainly in the region where

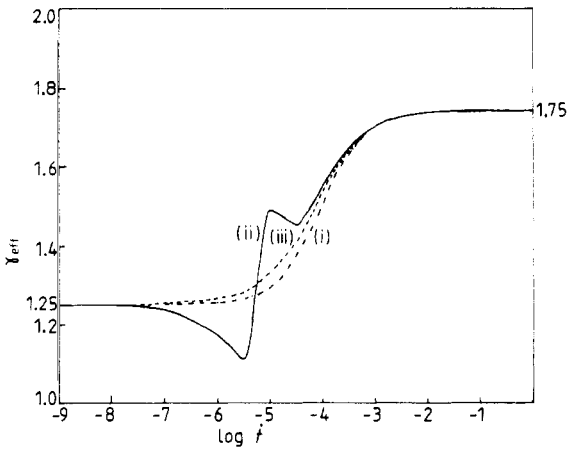


Figure 2. The effective exponent (see equation (33)) against $\log i$ for $g = 10^{-8}$ for the sc lattice for the three choices for $P(z)$, see equations (28) to (30).

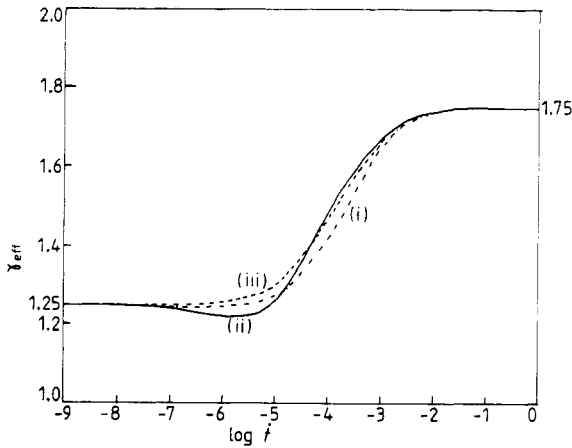


Figure 3. Same as figure 2 but for the FCC lattice.

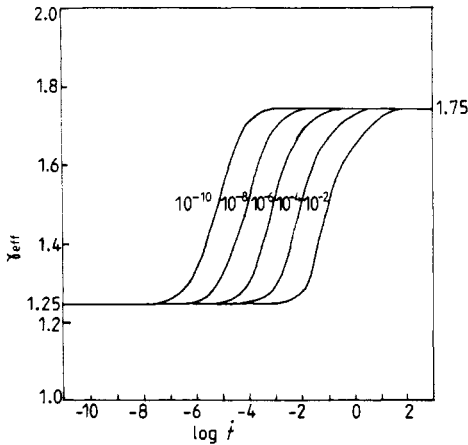


Figure 4. The effective exponent (see equation (33)) against $\log i$ for various values of g (given on curves) for the sc lattice. For $P(z)$, choice (i) is made (see equation (28)).

the anisotropic effects predominate. This may be due to our assumption of a simple behaviour (8) for the singularity of $X(x)$ near \dot{x} . In order to get better results in this region, one needs to estimate the function $P(z)$ more accurately near $z = 1$ (see remarks in the last paragraph of section VII B of PJF). We concentrate on the choice (i) because it gives smooth γ_{eff} and utilises the full series (26). In figures 4 and 5, we depict γ_{eff} against $\log t$ for various values of g for the two lattices. Since the critical region is usually for $t \leq 10^{-2}$, one should not take the graphs seriously beyond this reduced temperature.

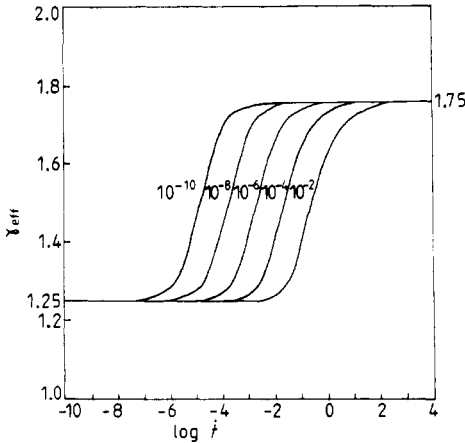


Figure 5. Same as figure 4 but for the FCC lattice.

This is because for $t \geq 10^{-2}$, there is expected to be a crossover to the mean-field exponent of unity. So, for $g \geq 10^{-8}$ (see the figures), one may not see a complete crossover to the isotropic value 1.75. Experiments in the range $g \geq 10^{-8}$ and $t \leq 10^{-2}$ may yield intermediate values of γ_{eff} . For $g \leq 10^{-8}$, however, our graphs predict a gradual crossover from 1.75 to 1.25 as one goes towards the critical temperature. Finally, it should be noted that the crossover region (suitably defined) is about four decades in t for a given value of g . Its length is practically independent of lattice type as it depends mainly on the crossover exponent φ .

6. Concluding remarks

We have studied the crossover behaviour of the susceptibility of quasi-two-dimensional Ising models. 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 the universal parameters. We have also constructed approximants for the scaling function valid in the whole critical region and presented plots of γ_{eff} against reduced critical temperature for a range of values of anisotropy for the SC and the FCC lattices.

In concluding, we remark that it would be highly desirable to study this model and

obtain the values of all the parameters using renormalisation group techniques, e.g., by following Bruce (1974) and by the recent partial differential approximant techniques (Fisher 1977a, b, Stilck and Salinas 1981).

Acknowledgments

We have benefited from correspondence with Professor M E Fisher during the initial stages of this work. One of us (WLB) acknowledges the award of a JRF by UGC (India) to her. Thanks are also due to Dr D K Ray of NEC for allowing us to use their computing facilities.

References

- Abe R 1970 *Prog. Theor. Phys.* **44** 339
 Barouch E, McCoy B M and Wu T T 1973 *Phys. Rev. Lett.* **31** 1409
 Basaiawmoit W L and Singh S 1982a *Phys. Lett.* **88A** 251
 ——— 1982b *Phys. Lett.* **89A** 313
 Bruce A D 1974 *J. Phys. C: Solid State Phys.* **7** 2089
 Cittert C A W and Kasteleyn P 1972 *Phys. Lett.* **42A** 143
 Coniglio A 1972 *Physica* **58** 489
 De Jongh L J 1976 *Physica* **82B** 247
 De Jongh L J and Miedema A R 1974 *Adv. Phys.* **23** 1
 De Jongh L J and Stanley H E 1976 *Phys. Rev. Lett.* **36** 817
 Domb C 1974 *Phase Transitions and Critical Phenomena* vol 3 ed. C Domb and M S Green (New York: Academic Press) p 464
 Enting I G and Oitmaa J 1971 *Phys. Lett.* **38A** 107
 Fisher M E 1967 *Rep. Prog. Phys.* **30** 615
 ——— 1977a *Statistical Mechanics and Statistical Methods in Theory and Applications* ed. U Laudman (New York: Plenum) p 3
 Fisher M E 1977b *Physica* **86–8B** 590
 Fisher M E and Jasnow D 1982 *Phase Transitions and Critical Phenomena* ed. C Domb and M S Green (New York: Academic Press) to be published
 Gaunt D S and Guttman A J 1974 *Phase Transitions and Critical Phenomena* vol 3, ed. C Domb and M S Green (New York: Academic Press) p 181
 Harbus F and Stanley H E 1973a *Phys. Rev. B* **7** 365
 ——— 1973b *Phys. Rev. B* **8** 2268
 Kouvel J S and Fisher M E 1964 *Phys. Rev.* **136A** 1626
 Kramers H A and Wannier G H 1941 *Phys. Rev.* **60** 252
 Krasnow R, Harbus F, Liu L L and Stanley H E 1973 *Phys. Rev. B* **7** 370
 Liu L L and Stanley H E 1972 *Phys. Rev. Lett.* **29** 927
 ——— 1973 *Phys. Rev. B* **8** 2279
 Navarro R and De Jongh L J 1978 *Physica* **94B** 67
 Oitmaa J and Enting I G 1971 *Phys. Lett.* **36A** 91
 ——— 1972 *Proc. Phys. Soc.* **5** 231
 Onsager L 1944 *Phys. Rev.* **65** 117
 Paul G and Stanley H E 1971 *Phys. Lett.* **37A** 347
 Pfeuty P, Jasnow D and Fisher M E 1974 *Phys. Rev. B* **10** 2088
 Rapaport D C 1971 *Phys. Lett.* **37A** 407
 Riedel E K and Wegner F J 1969 *Z. Phys.* **225** 195
 ——— 1974 *Phys. Rev. B* **9** 294
 Singh S 1975 *PhD Thesis* University of Pittsburgh, unpublished
 Singh S and Jasnow D 1975 *Phys. Rev. B* **11** 3445, **B 12** 493

- Stanley H E 1971 *Introduction to Phase Transitions and Critical Phenomena* (London: Oxford University Press)
- 1974 *Phase Transitions and Critical Phenomena* vol 3, ed. C Domb and M S Green (New York: Academic Press) p 493
- Stilck J F and Salinas S R 1981 *J. Phys. A: Math. Gen.* **14** 2027
- Suzuki M 1971 *Prog. Theor. Phys.* **46** 1054
- Sykes M F, Gaunt D S, Roberts P D and Wyles J A 1972 *J. Phys. A: Math. Gen.* **5** 624