

# Effect of Anisotropy on the Critical Behaviour of Three-Dimensional Heisenberg Ferromagnets

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The anisotropic nearest-neighbour Heisenberg model for the simple cubic lattice has been investigated by interpolating the anisotropy between the Ising and isotropic Heisenberg limits via general spin high-temperature series expansions of the zero-field susceptibility. This is done by estimating the critical temperature ( $T_c^{(3)}$ ) and the susceptibility exponent  $\gamma$  from the analysis of the series by the Ratio and Padé approximants methods. It is noted that  $T_c^{(3)}$  varies with anisotropy while  $\gamma$  is almost the same for the anisotropic system, and a jump in it occurs for the isotropic case in agreement with the universality hypothesis. The effect of anisotropy on the susceptibility is also shown. Further, it is seen that estimates of  $\gamma$  for the two extreme limits agree well with those of previous theoretical as well as experimental investigations. In addition, critical temperatures have been summarised in a relation, and expressions for the magnetisation have been derived.

## 1. Introduction

Critical indices (exponents) of the various physical quantities describe the nature and strength of their singularities and are, therefore, key parameters in characterising critical point phenomena. Because of this fact many investigations concerning the critical phenomena, both experimental and theoretical, have centred on the determination of the exponents. The determination of the exponents has also been motivated to confirm or to disprove the scaling and universality hypotheses<sup>1, 2</sup>. The Ising and Heisenberg models have, in particular, been chosen for such investigations because of their relevance to real ferro- and antiferromagnets, and also because they can be viewed as mathematically simple and physically very general forms of a classical and quantum mechanical many body problem. The series expansion method has proven to be the most fruitful technique to determine the various critical exponents for both the models on different lattices.

In both the models the occurrence of a phase transition is closely connected with the existence of spontaneous magnetisation. In the Ising model the one-dimensional (1-d) lattice does not exhibit a phase transition<sup>3</sup> but the two- and three-dimensional (2-d and 3-d) lattices have a phase transition<sup>4–6</sup>. On the other hand, in the Heisenberg model 1-d and 2-d lattices have no phase transition<sup>7</sup> while 3-d lattices have a phase transition<sup>8</sup>. Because of this fact much attention has been paid to the critical behaviour of 3-d Ising and Heisenberg models. It has been found<sup>9–11</sup> that the critical exponents are the same for all 3-d lattices in agreement with the universality belief.

Further, considerable efforts have been made in the last ten years to see the effect of change in the symmetry of the order parameter (change from an Ising to an isotropic Heisenberg system) on the critical behaviour. Dalton and Wood<sup>12</sup> have investigated the anisotropic nearest-neighbour (nn) Heisenberg model by analysing high-temperature series (HTS) of five terms for the zero field susceptibility for spin 1/2 by the Padé approximant method. Similar investigations have been presented by Jou and Chen<sup>13</sup> for spin 1/2 using seven terms series, and by Wood and Fox<sup>14</sup> for  $S=1/2, 1$  and  $3/2$  using six terms series. These workers have interpolated, with anisotropy, between the Ising and Heisenberg limits and concluded that the susceptibility exponent  $\gamma$  for 3-d cubic (bcc and fcc) lattices remains Ising like in the presence of anisotropy and increases discontinuously in the isotropic Heisenberg limit. This is in agreement with the conclusion drawn by Jasnow and Wortis<sup>15</sup> by analysing eight terms series of different physical quantities for the  $S=\infty$  anisotropic nn Heisenberg model for 3-d fcc lattice. In an investigation for the simple cubic (sc) lattice by Obokata et al.<sup>16</sup> for spin 1/2 no clear conclusion has been drawn. Hence we have investigated the anisotropic nn Heisenberg model for sc lattice by analysing general spin HTS<sup>17</sup> of six terms of the zero-field susceptibility. This is done by estimating the critical parameters by both the Ratio- and Padé-methods for comparison. These are discussed in the light of existing investigations. In addition transition temperatures are summarised in a relation, and expressions for the magnetisation are derived. The effect of anisotropy on the susceptibility is also shown.

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## 2. Theoretical Details and Results

written in the form<sup>17</sup>

### 2.1. High Temperature Zero-Field Susceptibility Series

The anisotropic Heisenberg spin Hamiltonian<sup>17</sup> for the present investigation may be given in the form

$$\mathcal{H} = -2J \sum_{ij} \{S_{iz} S_{jz} + 2\eta (S_{ix} S_{jx} + S_{iy} S_{jy})\} - \mu H \sum_{i=1}^N S_{iz}, \quad (1)$$

where  $\eta$  is the anisotropy parameter and the other symbols have their usual meaning. The Ising and isotropic Heisenberg models correspond to  $\eta = 0$  and  $\eta = 0.5$  respectively. The expansion of the zero field susceptibility  $\chi_0$ , corresponding to (1), can be

$$\frac{k_B T \chi_0}{\mu^2} = \frac{X}{3} \left\{ 1 + \sum_{n=1}^{\infty} a_n(\eta, X) K^n \right\}, \quad (2)$$

where  $X = S(S+1)$ ,  $K = JX/2k_B T$  and the other symbols have their usual meaning. The coefficients  $a_n$  (up to  $n=6$ ) have been calculated from the general formalism of Wood and Dalton<sup>17</sup> for the sc lattice for different values of  $S$  (i.e. for  $S=1/2, 1, 3/2, 2, 3$  and  $\infty$ ) in the range  $0 \leq \eta \leq 0.5$ . These are presented in Table 1.

### 2.2. Estimation of the Critical Temperature and Exponent

(a) Pade Approximant (PA) method : This is a very powerful method<sup>18</sup> to estimate the critical parameters from the truncated series. The

Table 1. The coefficients  $a_n$  of the expansion (2) for different values of  $S$  and  $\eta$ .

$S$	$\eta$	0.0	0.1	0.2	0.3	0.4	0.5
1	$a_1$	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
	$a_2$	53.33333	52.90667	51.62667	49.49333	46.50667	44.23111
	$a_3$	350.81481	345.12592	328.05925	299.61481	259.79259	208.59259
	$a_4$	2231.30864	2180.37665	2029.27976	1783.11522	1450.41383	1042.96296
	$a_5$	14162.38354	13744.89495	12523.17445	10589.45790	8097.47174	5262.43292
	$a_6$	88512.55583	84793.24530	76064.68280	61096.83753	43980.54564	24731.82401
1/2	$a_1$	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
	$a_2$	56.00000	55.73333	54.93333	53.60000	51.73333	49.33333
	$a_3$	389.33333	385.42222	373.68889	354.13333	326.75556	291.55556
	$a_4$	2623.11111	2584.66299	2469.31010	2277.02684	2007.77055	1661.48148
	$a_5$	17641.36294	17298.88838	16277.68070	14596.38803	12277.49080	9390.30125
	$a_6$	116995.67411	114186.29407	105945.24529	92504.08535	74346.00981	52053.74814
3/2	$a_1$	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
	$a_2$	56.74667	56.52480	55.85920	54.74986	53.19680	51.20000
	$a_3$	400.33090	396.99403	386.98340	370.29903	346.94091	316.90904
	$a_4$	2742.08490	2708.59435	2607.81163	2437.92604	2204.52959	1889.26736
	$a_5$	18752.29792	18448.27136	17536.33088	16016.90118	13890.68928	11158.65601
	$a_6$	126541.07222	124012.81650	116474.58410	104007.46590	86733.39001	64749.83489
2	$a_1$	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
	$a_2$	57.06667	56.86400	56.25600	55.24267	53.82400	52.00000
	$a_3$	405.07259	401.99206	392.75046	377.34779	355.78406	328.05926
	$a_4$	2794.33878	2763.18028	2669.30775	2511.41860	2287.49912	1994.61729
	$a_5$	19247.73696	18962.88896	18106.12455	16670.77890	14645.74438	12015.47059
	$a_6$	130867.99937	128479.44910	121326.51541	109414.61670	92724.14167	71152.75141
3	$a_1$	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
	$a_2$	57.33333	57.14667	56.58667	55.65333	54.34667	52.66667
	$a_3$	409.03704	406.17481	397.58839	383.27703	363.24148	337.48148
	$a_4$	2838.55767	2809.34912	2721.50464	2573.46424	2362.77856	2086.01848
	$a_5$	19669.62438	19402.05952	18595.31187	17237.20755	15307.46240	12777.67814
	$a_6$	134584.91551	132325.01801	125534.16008	114155.91955	98058.87120	76983.14200
$\infty$	$a_1$	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
	$a_2$	57.60000	57.42933	56.91733	56.06400	54.86933	53.33330
	$a_3$	413.01333	410.37369	402.45476	389.25653	370.77902	347.02222
	$a_4$	2883.12889	2856.14019	2774.62070	2636.91014	2440.24145	2180.74074
	$a_5$	20099.81194	19850.75110	19097.81133	17823.72150	15999.69325	13585.42786
	$a_6$	138405.06470	136286.53691	129896.56924	119119.74981	103723.14808	83296.21748

susceptibility series of the present investigation, near the critical point, may be defined by the relationship<sup>9, 19</sup>

$$\chi = A(1 - K/K_c)^{-\gamma}, \quad (3)$$

where  $\chi = 3 k_B T \chi_0 / \mu^2 X$ ,  $K_c = JX/2 k_B T_c^{(3)}$  ( $T_c^{(3)}$  stands for the temperature at which the susceptibility diverges for 3-d systems),  $A$  is the amplitude and  $\gamma$  the critical exponent. Estimates of  $K_c$  are obtained from the appropriate poles (zeros of the denominator) of the PA's to  $d(\ln \chi)/dK$ . The Pade analysis of  $d(\ln \chi)/dK$  for  $S=3$  with  $0 \leq \eta \leq 0.5$  is presented in Table 2. This table shows that estimates of  $K_c$  from higher order approximants are in good agreement with each other. Antiferromagnetic singularities  $K_1$  have also been estimated with a view to estimate  $K_c$  from the PA's to  $(K - K_1) d(\ln \chi)/dK$ . This procedure<sup>20, 21</sup> removes the antiferromagnetic singularities and improves the consistency in  $K_c$ . But the  $K_1$  were found irregular, which prevented us from doing such a refining. The estimates of  $\gamma$  are made from the values of the higher order PA's to  $(K_c - K) d(\ln \chi)/dK$

at  $K = K_c$ . These are presented in Table 3 for  $S=3$  in the range  $0 \leq \eta \leq 0.5$ . It has been seen that a change of 0.0005 in the value of  $K_c$  leads to a change of about 0.01 in the value of  $\gamma$ . The estimated  $K_c$  and  $\gamma$  from the higher order PA's to  $d(\ln \chi)/dK$  and  $(K_c - K) d(\ln \chi)/dK$  respectively for different values of  $S$  and  $\eta$  are presented in Table 4. The uncertainty limits, which are somewhat subjective, are also given in Table 4.

(b) Ratio Method: The estimates of  $K_c^{-1}$  are made by plotting square roots of the ratios of alternate coefficients as a function of  $1/n$  and extrapolating for  $n = \infty$ . This procedure<sup>18</sup> removes the antiferromagnetic singularities (causing oscillations in the ratios of the successive coefficients) and gives reliable estimates for all  $\eta$  ( $0 \leq \eta \leq 0.5$ ). An example for  $S=3$  is presented in Figure 1. The critical temperatures, thus estimated, are presented in Table 5. The estimates of  $\gamma$  are made from the sequences of the  $\gamma_n = (r_n K_{c1}^{-1} - 1)n + 1$  where  $r_n = a_n/a_{n-1}$ . These are also listed in Table 5. The inverse of  $K_c$  as a function of  $\eta$  for different spins is shown in Figure 2.

Table 2. Estimates of  $K_c$  for  $S=3$  with different values of  $\eta$  from the higher order Pade approximants to  $d(\ln \chi)/dK$ . \* Denotes the complex pole.

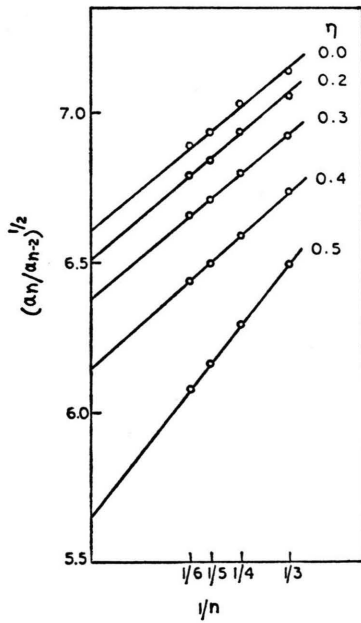
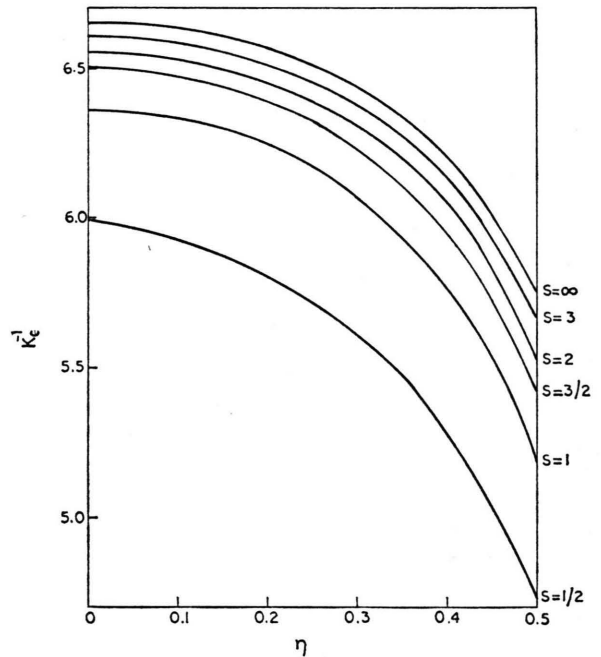
$D$	$N$	$\eta=0$		$D$	$N$	$\eta=0.1$		$D$	$N$	$\eta=0.2$	
	1	2	3		1	2	3		1	2	3
2	0.1489	0.1503	0.1508	2	0.1496	0.1507	0.1512	2	0.1515	0.1521	0.1527
3	0.1504	0.1512		3	0.1508	0.1518		3	0.1522	0.1540	
4	0.1509			4	0.1513			4	0.1527		
Estimates		0.1508 $\pm$ 0.0004				0.1512 $\pm$ 0.0005				0.1525 $\pm$ 0.0005	
		$\eta=0.3$				$\eta=0.4$				$\eta=0.5$	
2	0.1554	0.1552	0.1553	2	0.1620	0.1613	0.1614	2	0.1740	0.1744	0.1755
3	0.1560	*		3	*	0.1614		3	0.1743	0.1743	
4	0.1556			4	0.1614			4	0.1753		
Estimates		0.1654 $\pm$ 0.0005				0.1614 $\pm$ 0.0005				0.1747 $\pm$ 0.0008	

Table 3. Estimates of  $\gamma$  for  $S=3$  with different values of  $\eta$  from higher order Pade approximants to  $(K_c - K) d(\ln \chi)/dK$  at  $K=K_c$  (the values of  $K_c$  are taken from Table 2).

$D$	$N$	2	3	$D$	$N$	2	3	$D$	$N$	2	3
	1	$\eta=0$			1	$\eta=0.1$			1	$\eta=0.2$	
2	1.206	1.211	1.210	2	1.202	1.208	1.205	2	1.191	1.203	1.201
3	1.210	1.209		3	1.207	1.206		3	1.194	1.194	
4	1.210			4	1.208			4	1.201		
Estimates		1.21 $\pm$ 0.01				1.21 $\pm$ 0.01				1.20 $\pm$ 0.01	
		$\eta=0.3$				$\eta=0.4$				$\eta=0.5$	
2	1.188	1.187	1.189	2	1.211	1.214	1.215	2	1.333	1.340	1.334
3	1.188	1.189		3	1.212	1.213		3	1.336	1.334	
4	1.188			4	1.213			4	1.331		
Estimates		1.19 $\pm$ 0.01				1.21 $\pm$ 0.015				1.33 $\pm$ 0.02	

Table 4. Estimates of  $K_c$  (upper line) and  $\gamma$  (lower line) for various values of  $S$  and  $\eta$  from the higher order Pade approximants.

$S \quad \eta$	0	0.1	0.2	0.3	0.4	0.5
$\frac{1}{2}$	$0.1661 \pm 0.0007$	$0.167 \pm 0.001$	$0.170 \pm 0.002$	$0.178 \pm 0.003$	$0.185 \pm 0.005$	$0.21 \pm 0.02$
$\frac{1}{2}$	$1.25 \pm 0.02$	$1.24 \pm 0.02$	$1.23 \pm 0.02$	—	—	—
1	$0.1561 \pm 0.0005$	$0.1569 \pm 0.0005$	$0.1588 \pm 0.0007$	$0.1627 \pm 0.0007$	$0.171 \pm 0.001$	$0.192 \pm 0.001$
1	$1.24 \pm 0.01$	$1.24 \pm 0.01$	$1.23 \pm 0.01$	$1.22 \pm 0.02$	$1.24 \pm 0.02$	$1.38 \pm 0.03$
$\frac{3}{2}$	$0.1529 \pm 0.0005$	$0.1538 \pm 0.0005$	$0.1550 \pm 0.0005$	$0.1590 \pm 0.0006$	$0.1661 \pm 0.0006$	$0.182 \pm 0.001$
$\frac{3}{2}$	$1.23 \pm 0.01$	$1.23 \pm 0.01$	$1.22 \pm 0.01$	$1.21 \pm 0.015$	$1.23 \pm 0.015$	$1.36 \pm 0.02$
2	$0.1517 \pm 0.0005$	$0.1524 \pm 0.0005$	$0.1539 \pm 0.0005$	$0.1571 \pm 0.0005$	$0.1634 \pm 0.0006$	$0.178 \pm 0.001$
2	$1.22 \pm 0.01$	$1.22 \pm 0.01$	$1.21 \pm 0.01$	$1.20 \pm 0.015$	$1.22 \pm 0.015$	$1.34 \pm 0.02$
3	$0.1508 \pm 0.0004$	$0.1512 \pm 0.0005$	$0.1525 \pm 0.0005$	$0.1554 \pm 0.0004$	$0.1614 \pm 0.0005$	$0.1747 \pm 0.0008$
3	$1.21 \pm 0.01$	$1.21 \pm 0.01$	$1.20 \pm 0.01$	$1.19 \pm 0.01$	$1.21 \pm 0.015$	$1.33 \pm 0.02$
$\infty$	$0.1498 \pm 0.0004$	$0.1501 \pm 0.0005$	$0.1511 \pm 0.0005$	$0.1541 \pm 0.0005$	$0.1595 \pm 0.0005$	$0.1725 \pm 0.0008$
$\infty$	$1.20 \pm 0.01$	$1.20 \pm 0.01$	$1.20 \pm 0.01$	$1.19 \pm 0.01$	$1.21 \pm 0.015$	$1.33 \pm 0.02$

Fig. 1. The ratios  $(a_n/a_{n-2})^{1/2}$  of the susceptibility series plotted against  $1/n$  for  $S=3$  with different values of  $\eta$ .Fig. 2. Variation of the critical temperature with the anisotropy parameter  $\eta$  for different values of spin.Table 5. Estimates of  $K_c^{-1}$  (upper line) and  $\gamma$  (lower line) for various values of  $S$  and  $\eta$  from the ratio method.

$S \quad \eta$	0.0	0.1	0.2	0.3	0.4	0.5
$\frac{1}{2}$	5.99	5.94	5.82	5.57	5.33	4.74
$\frac{1}{2}$	$1.25 \pm 0.04$	$1.25 \pm 0.05$	$1.27 \pm 0.05$	$1.28 \pm 0.05$	—	—
1	6.36	6.33	6.25	6.08	5.78	5.19
1	$1.25 \pm 0.02$	$1.25 \pm 0.02$	$1.25 \pm 0.02$	$1.25 \pm 0.02$	$1.27 \pm 0.02$	$1.42 \pm 0.03$
$\frac{3}{2}$	6.50	6.46	6.40	6.24	5.96	5.43
$\frac{3}{2}$	$1.24 \pm 0.02$	$1.24 \pm 0.02$	$1.24 \pm 0.02$	$1.24 \pm 0.02$	$1.27 \pm 0.02$	$1.41 \pm 0.02$
2	6.55	6.52	6.45	6.32	6.07	5.55
2	$1.23 \pm 0.02$	$1.23 \pm 0.02$	$1.23 \pm 0.02$	$1.23 \pm 0.02$	$1.26 \pm 0.02$	$1.40 \pm 0.02$
3	6.61	6.59	6.51	6.38	6.15	5.66
3	$1.22 \pm 0.02$	$1.22 \pm 0.02$	$1.22 \pm 0.02$	$1.22 \pm 0.02$	$1.25 \pm 0.02$	$1.39 \pm 0.02$
$\infty$	6.65	6.63	6.56	6.45	6.22	5.76
$\infty$	$1.22 \pm 0.02$	$1.22 \pm 0.02$	$1.22 \pm 0.02$	$1.22 \pm 0.02$	$1.25 \pm 0.02$	$1.38 \pm 0.02$

Next,  $k_B T_c^{(3)}/J$  has been plotted as a function of  $X$  for different values of  $\eta$  ( $0 \leq \eta \leq 0.5$ ) in Figure 3. The remarkable feature of Fig. 3 is that

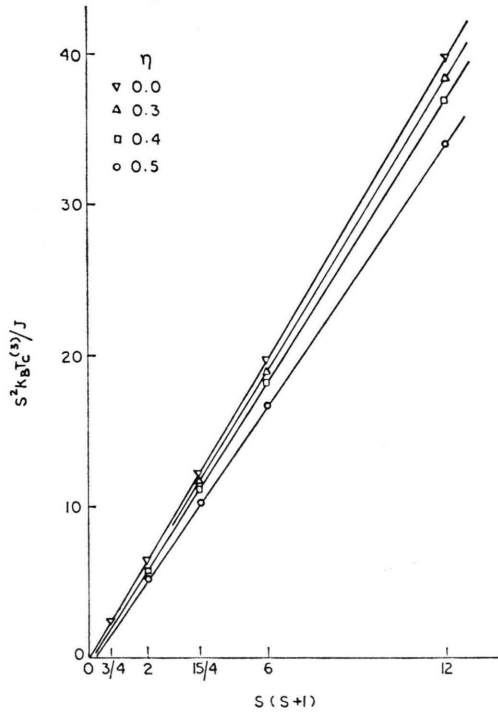


Fig. 3. Variation of  $k_B T_c^{(3)}/J$  with  $S(S+1)$ .

the critical points lie on straight lines for any  $\eta$  ( $0 \leq \eta \leq 0.5$ ). From this property the critical temperatures are summarised in the equation

$$k_B T_c^{(3)}/J \cong (3.33 - 3.6 \eta^3) \cdot [S(S+1) - (0.075 + 0.85 \eta^3)], \quad (4)$$

### 2.3. Estimation of $\chi$

The presence of interfering singularities prevented us from getting a reliable estimate of  $\chi$  as a function of temperature by the PA method. Therefore the estimation of  $\chi$  as a function of temperature (i.e.  $K^{-1}$ ) has been made by plotting  $\chi$  as a function of  $1/n$  and extrapolating for  $n = \infty$ . Results thus obtained for  $S=3$  with  $0 \leq \eta \leq 0.5$  are shown in Figure 4. Similar plots can be obtained for other spins.

### 2.4. Spin-Wave Results for Magnetisation

It is well known that the results of the spin-wave theory are excellent at low temperatures for practical purposes. With this view expressions for the magnetisation, valid for any spin for the sc lattice

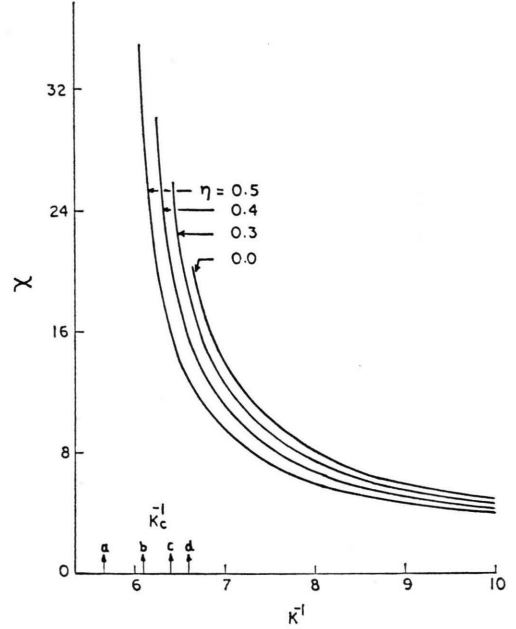


Fig. 4. The zero-field susceptibility as a function of the temperature for  $S=3$  with  $\eta$  as a parameter. The arrows  $a$ ,  $b$ ,  $c$ , and  $d$  indicate the critical temperatures  $K_c^{-1}$  (located from the ratio method corresponding to  $\eta=0.5, 0.4, 0.3$  and  $0.0$  respectively).

defined by the Hamiltonian (1), are derived by using the ideas of the spin-wave theory<sup>22, 23</sup>. For sufficiently low temperatures, the physical assumptions of the theory are: (i) there exists an ordered ground state characterised by a magnetisation in the  $z$  direction and (ii) deviations from the ordered ground state are small. Hence  $S_x \ll S$ ,  $S_y \ll S$  and  $S - S_z \ll S$  where  $S_x$ ,  $S_y$  and  $S_z$  are respectively the components of the classical spin  $S$  in the  $x$ ,  $y$  and  $z$  directions.

The magnetisation at low temperature is given by<sup>22</sup>

$$\bar{m} = S - \frac{V_0}{(2\pi)^d} \int_{BZ} n_k d\mathbf{k} \quad (5)$$

where the integral is over the Brillouin zone,  $V_0$  is the volume of a unit cell,  $d$  is the dimensionality and  $n_k$  is the wave occupation number.

Next, in order to get expressions for the magnetisation a set of dynamical equations for the spins were obtained using the ideas of the spin-wave theory and Hamiltonian (1). The set of linear equations, thus obtained, was reduced to an approximate set of linear equations by taking  $S_{jz} = S$  and neglecting terms of the order  $S_{ix} S_{jy}$  according to the assumptions of the theory. Further, the normal mode



frequencies (for each wave vector  $\mathbf{k}$ ) obtained by Fourier transformation of the reduced equations for simple cubic lattice, are given by

$$\omega_{\mathbf{k}} = h + 12JS \cdot \left[ 1 - \frac{2\eta}{3} (\cos k_x a + \cos k_y a + \cos k_z a) \right], \quad (6)$$

where  $h = \mu H$ . In the long wavelength limit Eq. (6) reduces to

$$\omega_{\mathbf{k}} = h + 12JS(1 - 2\eta) + 4JS\eta k^2 a^2. \quad (7)$$

Substituting the low temperature approximation to the wave occupation number ( $n_{\mathbf{k}} \cong k_B T / \omega_{\mathbf{k}} = 1 / \omega_{\mathbf{k}} \beta$ ) and the long wave length approximation to  $\omega_{\mathbf{k}}$  in (5), we get

$$\bar{m} = S - \frac{a^3}{2\beta\pi^2} \int_{k=0}^{k_m} k^2 dk \cdot \frac{k^2 dk}{h + 12JS(1 - 2\eta) + 4JS\eta k^2 a^2}. \quad (8)$$

Since at low temperatures the shape of the Brillouin zone is not important, the upper limit  $k_m$  may be defined by  $k_m = (2\pi/a)(3/4\pi)^{1/3}$ . Hence (8) reduces to

$$\bar{m} = S - \frac{1}{4\pi\eta JS\beta} \left( \frac{3}{4\pi} \right)^{1/3} + \frac{1}{16\pi^2\eta JS\beta} \sqrt{\frac{h + 12JS(1 - 2\eta)}{JS\eta}} \cdot \tan^{-1}(3)^{1/3} (4\pi)^{2/3} \sqrt{\frac{JS\eta}{h + 12JS(1 - 2\eta)}} \quad (6)$$

This expression is valid for all  $\eta$  except for  $\eta = 0$ . The  $\bar{m}$  for two extreme cases are given below.

Case (i): The expression for magnetisation for  $\eta = 1/2$  is given by

$$\bar{m} = S - \frac{1}{2\pi JS\beta} \left( \frac{3}{4\pi} \right)^{1/3}. \quad (10)$$

Case (ii): The expression for magnetisation for  $\eta = 0$  is given by

$$\bar{m} = S - \frac{1}{\beta(h + 12JS)}. \quad (11)$$

### 3. Discussion and Conclusions

(i) Figure 2 shows that  $K_c^{-1}$  (i.e.  $T_c^{(3)}$ ) is finite and spin dependent for all values of  $\eta$  ( $0 \leq \eta \leq 0.5$ ). It decreases as  $\eta$  increases slowly near the Ising limit and rapidly near the isotropic limit for each

spin. The curves are qualitatively similar to the curve for  $S = \infty$  of the anisotropic nn Heisenberg model for 3-d fcc lattice<sup>15</sup>. The cause of this type of variation of the critical temperature with  $\eta$  is clear from the Hamiltonian (1). It can be seen from (1) that if  $\eta < 0.5$ , the relative probability of the spin to become parallel to the  $z$  axis is larger than to be in the  $xy$  plane. Therefore the critical temperature is higher for smaller  $\eta$ .

(ii) The behaviour of the exponent  $\gamma$ , as  $\eta$  varies from the Ising limit towards the isotropic Heisenberg limit, is of special interest. Table 4 shows that  $\gamma$  for  $S > 1/2$ , is Ising like in presence of anisotropy and a jump in it occurs for the isotropic case. A similar trend of  $\gamma$  is clear from Table 5 also. The minor anomaly in the ratio estimates of  $\gamma$  near the isotropic limit is due to the presence of isotropic behaviour and the short series effects. Thus the behaviour of  $\gamma(\eta)$  for  $S > 1/2$ , is in agreement with the universality belief in accordance with the previous investigations on the cubic lattices<sup>12-15a</sup>. It is remarkable to note that estimates of  $\gamma$  from the Pade method are lower than those from the ratio method. This is because of the fact that estimates of  $K_c$  by the Pade method are lower than those from the ratio method by upto 0.3 to 2%. However, estimates of  $\gamma$  by the ratio method for the Ising and isotropic Heisenberg limits are in good agreement with those obtained from the Pade and ratio methods using longer series<sup>24-26</sup>. Hence, critical parameters from the ratio method seem more reliable for all  $\eta$  ( $0 \leq \eta \leq 0.5$ ) than those obtained from the Pade method. Equation (4) can be used to locate critical temperatures for any set of  $S$  ( $\frac{1}{2} \leq S \leq \infty$ ) and  $\eta$  ( $0 \leq \eta \leq 0.5$ ). Although Fig. 2 can be used for the same purpose; its use is limited to those spins which are given in it.

The mean of the experimental values<sup>27</sup> of  $\gamma$  for the 3-d Heisenberg ferromagnets is known to be  $1.35 \pm 0.04$ . This is somewhat lower than the present ratio estimate. This difference is due to presence of anisotropy in the compounds. The experimental value<sup>27</sup> of  $\gamma$  (i.e.  $1.24 \pm 0.03$ ) for 3-d Ising compounds agrees also well with the present estimate.

(iii) Figure 4 shows how the susceptibility  $\chi$  depends upon anisotropy. It is clear that  $\chi$  is very sensitive to large  $\eta$  (i.e. small anisotropy) at low temperature and less sensitive to it for  $T \gg T_c^{(3)}$ .

(iv) Finally, we wish to mention that expressions, (9), (10) and (11) can be used for practical pur-

poses at low temperatures by making use of the relation  $\alpha = H_A/H_E = 1 - 2\eta$  (where  $\alpha$  is the anisotropy which can be determined experimentally,  $H_A$  is the anisotropy field and  $H_E$  the exchange field).

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- <sup>1</sup> R. B. Griffiths, Phys. Rev. Lett. **24**, 1479 [1970].
- <sup>2</sup> A. Hankey and H. E. Stanley, Phys. Rev. **B 6**, 3515 [1972].
- <sup>3</sup> M. E. Baur and L. H. Nosanow, J. Chem. Phys. **37**, 153 [1962].
- <sup>4</sup> C. N. Yang, Phys. Rev. **85**, 808 [1952].
- <sup>5</sup> R. Peierls, Proc. Cambridge Phil. Soc. **32**, 477 [1936].
- <sup>6</sup> R. B. Griffiths, J. Math. Phys. **8**, 478 [1967].
- <sup>7</sup> N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 [1966].
- <sup>8</sup> T. Oguchi, J. Phys. Soc. Japan **30**, 988 [1971].
- <sup>9</sup> M. E. Fisher, Rep. Prog. Phys. **30**, 615 [1967].
- <sup>10</sup> C. Domb, Adv. Physics **19**, 339 [1970].
- <sup>11</sup> R. G. Bowers and M. E. Woolf, Phys. Rev. **177**, 917 [1969].
- <sup>12</sup> N. W. Dalton and D. W. Wood, Proc. Phys. Soc. **90**, 459 [1967].
- <sup>13</sup> D. C. Jou and H. H. Chen, J. Phys. **C 6**, 2713 [1973].
- <sup>14</sup> D. W. Wood and P. F. Fox (to be published).
- <sup>15</sup> D. Jasnow and M. Wortis, Phys. Rev. **176**, 739 [1968].
- <sup>15a</sup> P. Pfeuty, D. Jasnow, and M. E. Fisher, Phys. Rev. **B 10**, 2088 [1974].
- <sup>16</sup> T. Obokata, I. Ono, and T. Oguchi, J. Phys. Soc. Japan **23**, 516 [1967].
- <sup>17</sup> D. W. Wood and N. W. Dalton, J. Phys. **C 5**, 1675 [1972].
- <sup>18</sup> D. L. Hunter and G. A. Baker, Jr., Phys. Rev. **B 7**, 3346 [1973].
- <sup>19</sup> H. E. Stanley, Introduction to Phase Transitions and Critical Phenomena, Clarendon, Oxford, England 1971, p. 90.
- <sup>20</sup> K. Pirnie, P. J. Wood, and J. Eve, Mol. Phys. **11**, 551 [1966].
- <sup>21</sup> R. Shanker and R. A. Singh, Indian J. Pure and Appl. Phys. **12**, 589 [1974].
- <sup>22</sup> R. E. Watson, M. Blume, and G. H. Vineyard, Phys. Rev. **181**, 811 [1969].
- <sup>23</sup> C. Kittel, Introduction to Solid State Physics, John Wiley, New York 1966, p. 464.
- <sup>24</sup> J. P. Van Dyke and W. J. Camp, Phys. Rev. **B 9**, 3121 [1974].
- <sup>25</sup> W. J. Camp and J. P. Van Dyke (to be published).
- <sup>26</sup> D. S. Ritchie and M. E. Fisher, Phys. Rev. **B 5**, 2668 [1972].
- <sup>27</sup> L. J. de Jongh and A. R. Miedema, Adv. Physics **23**, 1 [1974].