

Description of the Magnetic Properties of Linear Polymetallic Chains of Antiferromagnetically Coupled Atoms: An Analysis of the Equation and the Models used to describe Magnetic Susceptibility

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Experimental magnetic-susceptibility data presently available for a wide variety of compounds of copper(II), titanium(III), and oxovanadium(IV), which are thought to consist of infinite linear chains of coupled atoms, have been analysed with four equations obtained from the Ising and the Heisenberg models. The results lead to the emphatic conclusion that the anisotropic equations for the parallel and perpendicular components of the magnetic susceptibility which are obtained from the Ising model are quite inappropriate for the description of these compounds. In contrast, the equation for the parallel component may be used in isolation for the reasonable fitting of data, although this procedure cannot be theoretically justified. Two equations based on the isotropic Heisenberg model, which is universally applied to small finite systems, have been investigated. Unfortunately, these equations are empirical rather than analytical. One is based on the exact machine calculations of Bonner and Fisher for rings of 10 and 11 coupled atoms, and the second equation is based on the present Monte-Carlo calculations on open chains of 100 and 101 atoms. Although these equations differ considerably at low temperatures, both offer a useful basis for fitting the available experimental data. In particular, the empirical equations are valuable comparative tests for the validity of moderately successful analytical equations and thus provide an improved basis for drawing structural conclusions from magnetic-susceptibility data.

THE literature concerned with the magnetic properties of finite polymetallic systems is extensive and there is still a measure of controversy over the optimum description of these systems.¹⁻³ However, it is probably fair to comment that few advances in the description of finite clusters have occurred since the work of Bleaney and Bowers in 1952,⁴ whereas there has so far been no comparable success in the description of infinite systems. This value judgement is based on two main criteria, namely the derivation of an analytical equation from the model used to describe the system and, secondly, a good fit between observed data and the theoretical equation for reasonably pure, crystallographically characterised, compounds. To meet the second criterion it is desirable that the theoretical equation should incorporate few disposable parameters and, preferably, no more than one. This disposable parameter is usually the quantity described as the exchange integral, J . The basis of the Bleaney and Bowers method is to imagine a dipolar coupling of the form $-J_{ij}S_iS_j$ to exist between electrons formally assigned to the atoms i and j , where S_i and S_j represent spin quantum numbers. This type of expression neatly generates combined states which are quantised in the possible values of the total-spin quantum number.

In this work attention is restricted to chains composed of atoms with a formal complement of one unpaired

electron. The diversity of the compounds of interest may be conveniently indicated by mentioning some for which infinite linear chains have been established crystallographically, namely anhydrous copper(II) bromide,⁵ $K[CuF_3]$,^{6,7} the 1:1 copper(II) chloride-1,2,4-triazole complex,⁸ α - $[CuBr_2(NH_3)_2]$,⁹ $[Cu(CO_3)(NH_3)_2]$,¹⁰ diacetatocopper(II)-bis(*p*-toluidine) trihydrate,¹¹ copper(II) benzoate trihydrate,¹² the 1:1 complex of copper oxalate and ammonia,¹³ diammineoxalatocopper(II) dihydrate,¹⁴ α -bis(*N*-methylsalicylideneiminato)copper(II),¹⁵ and [bis(1,2-diphenylphosphino)ethane]dichlorocopper(II).¹⁶ It is relevant that not only are there very few known complexes of this type with strong intermetallic bonding¹⁷ but indeed only a handful of complexes are known with even the moderate interactions typical of many well characterised finite polymetallic complexes. This is because the Ising model has been fairly generally accepted until now as the most convenient basis for the interpretation of infinite linear-chain systems.^{18,19} Unfortunately, the defects of the Ising model are not manifest obviously when the coupling is weak,^{20,21} and many other workers now seriously doubt the validity of the model.^{22,23}

The Ising model is anisotropic because it involves the simplification of the effective spin-exchange Hamiltonian [equation(1)] by setting $\gamma = 0$.²⁴ With this simplification

¹ R. W. Jotham and S. F. A. Kettle, *Inorg. Chem.*, 1970, **9**, 1390.

² R. W. Jotham, S. F. A. Kettle, and J. A. Marks, *J.C.S. Dalton*, 1972, 428.

³ R. W. Jotham, S. F. A. Kettle, and J. A. Marks, *J.C.S. Faraday II*, 1976, 125.

⁴ B. Bleaney and K. D. Bowers, *Proc. Roy. Soc.*, 1952, **A214**, 451.

⁵ L. Helmholz, *J. Amer. Chem. Soc.*, 1947, **69**, 886.

⁶ A. Okazaki, *J. Phys. Soc. Japan*, 1969, **27**, 518.

⁷ H. Ikeda and K. Hirakawa, *J. Phys. Soc. Japan*, 1973, **35**, 722.

⁸ J. A. J. Jarvis, *Acta Cryst.*, 1962, **15**, 964.

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¹¹ R. C. Komson, A. T. McPhail, F. E. Mabbs, and J. K. Porter, *J. Chem. Soc. (A)*, 1971, 3447.

¹² H. Koizumi, K. Osaki, and T. Watanabe, *J. Phys. Soc. Japan*, 1963, **17**, 117.

¹³ L. Cavalca, A. Chiesi Villa, A. Gaetani Manfredotti, A. Mangia, and A. A. G. Tomlinson, *J.C.S. Dalton*, 1972, 391.

¹⁴ J. Garaj, H. Langfelderova, G. Lundgren, and J. Gažo, *Coll. Czech. Chem. Comm.*, 1972, **37**, 3181.

¹⁵ E. C. Lingafelter, G. L. Simmons, B. Morosin, E. Scheringer, and C. Freiburg, *Acta Cryst.*, 1961, **14**, 1222.

¹⁶ M. Mathew and G. J. Palenik, *Inorg. Chim. Acta*, 1971, **5**, 573.

¹⁷ T. W. Thomas and A. E. Underhill, *Chem. Soc. Rev.*, 1972, **1**, 99.

¹⁸ P. W. Ball, *Co-ordination Chem. Rev.*, 1969, **4**, 361.

¹⁹ E. Sinn, *Co-ordination Chem. Rev.*, 1970, **5**, 313.

²⁰ R. W. Jotham, *J.C.S. Chem. Comm.*, 1973, 178.

²¹ R. W. Jotham, *Phys. Stat. Solidi*, 1973, **B55**, K125.

²² S. Emori, M. Inoue, and M. Kubo, *Bull. Chem. Soc. Japan*, 1972, **45**, 2259.

²³ R. P. Eckberg and W. E. Hatfield, *J.C.S. Dalton*, 1975, 1365.

²⁴ G. F. Newell and E. W. Montroll, *Rev. Mod. Phys.*, 1953, **25**, 353.

ation Fisher obtained the analytical equations (2) and (3) (where $K = |J/4kT|$) for the parallel and perpendicular components of the molecular susceptibility.²⁵ (The

$$\mathcal{H} = -J_{ij}\{S_{i(z)}S_{j(z)} + \gamma[S_{i(x)}S_{j(x)} + S_{i(y)}S_{j(y)}]\} \quad (1)$$

symbols take their conventional meaning in these equations.) This practice contrasts significantly with the methods used for finite systems in which γ is set equal to

$$\chi_{||}' = (Ng^2\beta^2/4kT)\exp(J/2kT) + N\alpha \quad (2)$$

$$\chi_{\perp}' = (Ng^2\beta^2/4kT)\{[(\tanh K)/K] + \operatorname{sech}^2 K\} + N\alpha \quad (3)$$

unity (the Heisenberg model). The predictions of the Heisenberg and Ising models for the simple case of a typical copper(II) dimer are illustrated in Figure 1.

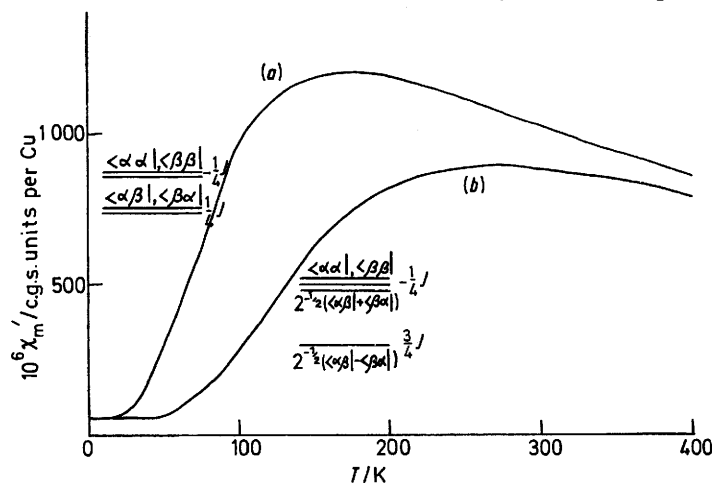


FIGURE 1 Predictions of Ising (a) and Heisenberg models (b) for the magnetic properties of a copper(II) dimer. $g = 2.16$, $J = -300 \text{ cm}^{-1}$, $10^6 N\alpha = 60 \text{ c.g.s. units per Cu}$

These predictions are strikingly different and, in practice, only the Heisenberg model is adequate for the description of known compounds of this type. Machine calculations on rings with up to 11 members have been carried out by Bonner and Fisher²⁶ using different values of γ . This is a much neglected paper, for it demonstrates that the predictions of the Ising and Heisenberg models do not converge appreciably as chain-length increases and, secondly, it provides some empirical data for the approximate description of infinite linear chains with the preferred model of Heisenberg. I have fitted these data, after modification to be consistent with equation (1), to the polynomial expression given in equation (4) where $P = kT/|J|$. (The reader should note that, although the polynomial fits the published data to better than 1%, it cannot be used for positive values of J .)

$$\chi_{m}' = (Ng^2\beta^2/|J|)(0.092281 + 0.18616P - 0.20556P^2 + 0.074679P^3 - 0.0091808P^4) + N\alpha \quad (4)$$

A reliable equation for the description of the magnetic susceptibility of linear-chain systems is urgently needed

²⁵ M. E. Fisher, *J. Math. Phys.*, 1963, **4**, 124.

²⁶ J. C. Bonner and M. E. Fisher, *Phys. Rev.*, 1964, **A135**, 640.

²⁷ D. B. Losee, H. W. Richardson, and W. E. Hatfield, *J. Chem. Phys.*, 1973, **59**, 3600.

²⁸ M. E. Fisher, *Amer. J. Phys.*, 1964, **32**, 343.

to facilitate the use of magnetic data as a criterion of structure. Empirical equations provide a basis against which the validity of any analytical equation may be tested as well as a coarse means of determining the exchange parameter, J , in appropriate cases. The urgent need to switch to the Heisenberg model is further emphasised by the fact that single-crystal susceptibility data on well defined linear complexes like copper(II) nitrate-pyrazine do not reveal the marked anisotropy predicted by the Ising model.²⁷ Fisher²⁸ in fact solved the problem analytically in the classical limit of infinite spin, but this work is of limited value since the results bear little resemblance to the calculations on moderately long chains or rings of finite spin²⁹⁻³² or, indeed, to experimental data. Fortunately, it is also possible to calculate the zero-

temperature value of the susceptibility for the case when $S = \frac{1}{2}$ in the Heisenberg model. Bonner and Fisher adopted the value $|J|\chi/Ng^2\beta^2 = 1/\pi^2 = 0.1014$, following fairly rigorous work by Griffiths which improved on earlier but similar approximations.³³⁻³⁵

Certain problems related to the work of Bonner and Fisher remain, however. First, it has been suggested that any linear antiferromagnetic chain of coupled spins is unstable with respect to a lattice distortion which dimerises the chain into an alternating antiferromagnet.³⁶ Duffy and Barr³⁷ provided empirical data for alternating antiferromagnetic chains, but I reject this approach except in cases where it is indicated by structural data, since the introduction of a second exchange parameter must reduce the ability of the model to discriminate one

²⁹ C. K. Majumdar, V. Mubayi, and C. S. Jain, *Chem. Phys. Letters*, 1973, **21**, 175; C. K. Majumdar, K. Krishnan, and V. Mubayi, *J. Phys. (C)*, 1972, **5**, 2896.

³⁰ H. P. Van de Braak and W. J. Caspers, *Phys. Stat. Solidi*, 1969, **35**, 933.

³¹ A. Earnshaw, B. N. Figgis, and J. Lewis, *J. Chem. Soc. (A)*, 1966, 1656.

³² S. Katsura, *Phys. Rev.*, 1962, **127**, 1508.

³³ R. B. Griffiths, *Phys. Rev.*, 1964, **A133**, 760.

³⁴ L. Hulthén, *Arkiv. Mat. Astron. Fysik*, 1938, **A26(11)**, 78.

³⁵ S. Inawashiro and S. Katsura, *Phys. Rev.*, 1965, **A140**, 892.

³⁶ G. Beni and P. Pincus, *J. Chem. Phys.*, 1972, **57**, 3531.

³⁷ W. Duffy, jun., and K. P. Barr, *Phys. Rev.*, 1968, **165**, 647.

structural type from another. A second difficulty in the whole-hearted adoption of the empirical data of Bonner and Fisher relates to the detailed values of calculated magnetic susceptibilities at low temperatures.²⁶ To illustrate this point, I have reproduced in Figure 2 the

chain in which the spin value at each magnetic centre is decided by reference to a random number and to the estimated probability that the centre should be aligned parallel with its neighbours. The total spin value for the chain is determined at the end of each walk and the mag-

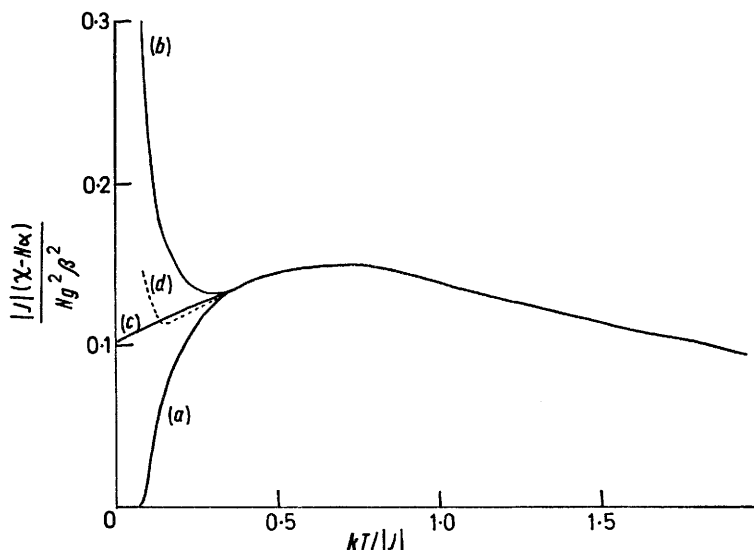


FIGURE 2 Calculated magnetic properties of rings of copper(II) ions containing 10 and 11 members (reproduced from ref. 26): (a) ten-membered ring; (b) eleven-membered ring; (c) recommended for infinite system; (d) average of (a) and (b)

data presented in their Figure 14. It is apparent that, at higher values of $kT/|J|$, the susceptibility curves for rings (and chains) of different lengths converge well to the estimated limit for infinite rings. However, this seems to be much more crudely approximated at low values of $kT/|J|$. It is particularly striking that the average susceptibility for rings of 10 and 11 members dips noticeably below the curve giving Bonner and Fisher's estimated values for an infinite ring and, moreover, this dip is itself more pronounced than that corresponding to the average susceptibility for rings of nine and 10 members.

There is clearly cause to suspect the estimated data of Bonner and Fisher at low values of $kT/|J|$ and to recognise that calculations on longer chains might reveal a very pronounced 'dip' in this region. I considered that it might be possible to deal with much longer chains through a Monte-Carlo type of calculation. In essence my calculation involved numerous 'walks' along the

* For example, in a linear trimer only the states $|\alpha\alpha\alpha\rangle$, $|\alpha\alpha\beta\rangle$, $|\beta\beta\alpha\rangle$, and $|\beta\beta\beta\rangle$ involve a parallel alignment of spins on centres 1 and 2. The first and last are components of the quartet state at energy $-\frac{1}{2}J$ but the others are scrambled among $M_s = \pm\frac{1}{2}$ components of the quartet and the two doublets D_1 and D_2 at energy 0 and J respectively. Thus, for the $M_s = \pm\frac{1}{2}$ components:

$$\begin{aligned} |Q^{\pm}\rangle &= 3^{-1}(|\alpha\alpha\beta\rangle + |\alpha\beta\alpha\rangle + |\beta\alpha\alpha\rangle) \\ |D_1^{\pm}\rangle &= 2^{-1}(|\alpha\alpha\beta\rangle - |\beta\alpha\alpha\rangle) \\ |D_2^{\pm}\rangle &= 6^{-1}(2|\alpha\beta\alpha\rangle - |\alpha\alpha\beta\rangle - |\beta\alpha\alpha\rangle) \end{aligned}$$

whence $|\alpha\alpha\beta\rangle = 6^{-1}(2|Q^{\pm}\rangle + 3|D_1^{\pm}\rangle - |D_2^{\pm}\rangle)$

It is now clear that the probability of the spins being aligned parallel on centres 1 and 2 is given by the sum of the populations of $|Q^{\pm}\rangle$, $\frac{1}{3}|D_1^{\pm}\rangle$, and $\frac{1}{6}|D_2^{\pm}\rangle$, i.e.:

$$P_{\text{trimer}} = \frac{8 + 3\exp(-J/2kT) + \exp(-3J/kT)}{6[2 + \exp(-J/2kT) + \exp(-3J/2kT)]} \quad (6a)$$

netic susceptibility may then be computed from statistical averages of a large number of walks along the same chain. Thus, if the probability of the total spin having the value M_i is found to be C_i at a temperature T for a chain of length L , the molecular susceptibility per centre is given by equation (5). It was convenient to utilise *ca.*

$$\chi_m' = (Ng^2\beta^2/LkT)(\sum C_i M_i^2) + N\alpha \quad (5)$$

10 000 random numbers in a single computer run for each of 15 temperatures, so that a statistical average of 100 chains of length 100 could form the basis for the calculation of magnetic susceptibility.

For a copper(II) dimer with a singlet state at $\frac{3}{4}J$ and a triplet state at $-\frac{1}{4}J$, the probability, P , that the spin will be aligned parallel is given by equation (6). Correspond-

$$P = \frac{2}{3 + \exp(-J/kT)} \quad (6)$$

ing expressions for longer chains are much more difficult to obtain, but it can be shown that equation (6) does not apply to every polymer* and does not lead to a perfect simulation of data calculated from the energy levels and the analytical equations for these systems.³⁸⁻⁴⁰ However, the situation improves markedly as the chain length increases and the data of Bonner and Fisher for rings of 10 and 11 members are reproduced reasonably well using the values of P given by equation (6), as shown in Table 1.

³⁸ A. Earnshaw, 'Introduction to Magnetochemistry,' Academic Press, New York, 1968.

³⁹ R. W. Jotham and S. F. A. Kettle, *Inorg. Chim. Acta*, 1970, **4**, 145.

⁴⁰ B. S. Tsukerblat and A. V. Ablov, *Zhur. strukt. Khim.*, 1971, **12**, 436.

This preliminary result encouraged me to use the value of P from equation (6) for chains of length 100 and 101

TABLE I

Calculated susceptibility data for chains of copper(II) ions^a

T/K	Cu ₁₀₀ , Cu ₁₀₁ average		Cu ₁₀₀ ^c	Cu ₁₀₁	Cu ₁₀₀ , Cu ₁₀₁ average ^e
	b	c			
0	471		60	∞	
30	489	723	60	204	132
60	523	402	80	134	107
120	585	423	282	270	276
180	628	579	457	489	473
210	642	627	548	548	548
240	652	659	593	584	589
270	656	675	602	625	613
300	654	682	645	637	641
330	650	682	615	633	624
360	640	665	630	625	627
390	631	665	604	606	605
420	618	643	621	601	611
480	595	623	570	554	562
600	540	553	550	550	550

^a All the susceptibility data in c.g.s. units per Cu. $g = 2.16$, $J = -300 \text{ cm}^{-1}$, $10^6 N\alpha = 60$ c.g.s. units per Cu. ^b Calculations of Bonner and Fisher for rings of copper(II) ions. ^c Calculations based on the probability value in equation (6). ^d The data have not been smoothed to give an indication of the random scatter.

and the data for these chains are also presented in Table I. ('Standard' values of $g = 2.16$, $10^6 N\alpha =$ c.g.s. units per Cu, and $J = -300 \text{ cm}^{-1}$ were used throughout the

temperature, I included the previously discussed value for $T = 0$ and the high-temperature data of Bonner and Fisher.²⁶ The resulting curve was too complicated to be conveniently described by a simple polynomial, but a Morse curve of the form (7) gave excellent agreement with

$$y = 0.096 \left(\left\{ 1 - \exp \left[-3.55 \left(\frac{kT}{|J|} - 0.25 \right) \right] \right\}^2 - 1 \right) \quad (7)$$

the differences between the values of $|J|(\chi - N\alpha)$ calculated from the simple equation (2) and those presented in Figure 3. Thus, the best empirical equation for the susceptibility of infinite linear chains of antiferromagnetically coupled chains of copper(II) ions based on my calculations takes the form presented in equation (8) where $P = kT/J$.

$$\chi_m' = \frac{Ng^2\beta^2}{|J|} \left[\frac{\exp(1/2P)}{4|P|} \right] + 0.096 \{ (1 - \exp[-3.55(|P| - 0.25)])^2 - 1 \} + N\alpha \quad (8)$$

I attempted to compare four possible models by applying the analytical and empirical equations to the fitting of experimental susceptibility data on possible linear-chain systems and to related compounds, including a number of dimers. The models used were: (a) the Ising model [equations (2) and (3) combined]; (b) the parallel component of the Ising model [equation (2) only]; (c)

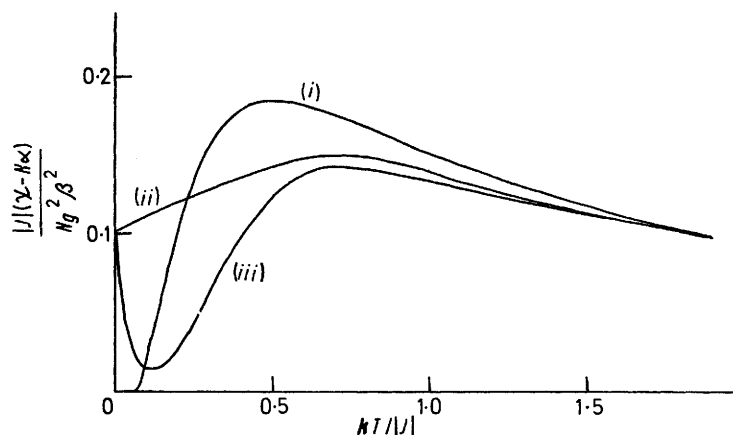


FIGURE 3 Calculated magnetic properties for three models of infinite chains of antiferromagnetically coupled copper(II) ions: (i) model (b) {the parallel component of the Ising model [equation (2)]}; (ii) model (c) {Bonner and Fisher's calculation [equation (4)]}; and (iii) model (d) {the Monte-Carlo calculation [equation (8)]}

calculations of susceptibility-temperature data.) Bonner and Fisher's data refer to rings, whereas my calculations are based on open chains. In general, rings have lower susceptibility values than open chains at higher temperatures, but these differences become slight as the chain length increases. The average values of $|J|(\chi - N\alpha)/Ng^2\beta^2$ for chains of 100 and 101 members are plotted in Figure 3 as a function of $kT/|J|$. (This format is particularly convenient for demonstrating the difference in the predictions of various models.) The data condensed into equation (4) are also plotted in Figure 3.

In order to calculate an empirical equation from our results which could be applied over an extensive range of

Bonner and Fisher's calculation [equation (4)]; (d) the Monte-Carlo calculation [equation (8)]; and (e) a simple dimer model [equation (9)]. The results of these calcul-

$$\chi_m' = \frac{Ng^2\beta^2}{kT} \left[\frac{\exp(J/kT)}{1 + 3 \exp(J/kT)} \right] + N\alpha \quad (9)$$

ations are presented in Supplementary Publication No. SUP 21938 (7 pp.),* together with structural information suggested by the original workers. The compounds investigated spanned many diverse types, including a variety of copper carboxylates and dicarboxylates and

* For details see Notices to Authors No. 7, *J.C.S. Dalton*, 1976, Index issue (items less than 10 pp. are supplied as full-size copies).

their derivatives,^{11,13,41-51} copper halides and their derivatives,⁵²⁻⁶¹ other copper(II) compounds,^{50,62-68} and some titanium(III) and oxovanadium(IV) complexes.⁶⁹⁻⁷⁴ For most of the copper(II) compounds the value of g was set at 2.16 if e.s.r. data were not available and $10^6 N\alpha$ was set at 75 c.g.s. units per Cu in this analysis. In the case of the d^1 complexes, corresponding values of $g = 1.96$ and $10^6 N\alpha = 40$ c.g.s. units per metal were used. Optimum models for each compound were selected from the results in SUP 21938, and used to compile the summary in Table 2. An optimum case is regarded as one in which the

TABLE 2
Summary of the optimum model data presented in
SUP 21938

Model	Number of optimum cases ^a		
	All compounds ^b	$10^6\sigma < 100$ c.g.s. units per metal	$10^6\sigma < 50$ c.g.s. units per metal
Ising	6.16	3.94	1.33
Ising (parallel component)	36.50	26.25	15.84
Bonner and Fisher	25.25	23.50	12.84
Monte Carlo	14.16	10.25	7.00
Dimer	26.94	25.06	18.00
Total cases	109	89	55

^a Ambiguous data are shared between the appropriate models. ^b Copper chloride methoxide and bromide methoxide appear in two sections of SUP 21938. Different sets of data on the same compound are counted separately.

value of the standard deviation, σ , does not exceed the smallest value for that compound by more than 20%, since I have previously shown that such a degree of variation might follow merely from a reasonable but incorrect choice of other parameters like g and $N\alpha$.²

The abject failure of the Ising model to describe the properties of compounds with a moderately strong antiferromagnetic coupling emerges clearly from Table 2 and I strongly recommend that the use of this model should be discontinued. The other three models of infinite linear systems appear to perform with comparable suc-

cess, although the data in Table 2 suggest that my own calculated equation is perhaps the least successful in fitting the susceptibility data. The relative success of model (b) is particularly encouraging because of the simple form of equation (3), but the models which use empirical data are relatively more successful when the compounds for which the data do not fit any model particularly well are disregarded.

The differences in the predictions of the three models (b)—(d) can be seen clearly from Figure 3. Bonner and Fisher's calculation differs most significantly from the other two at low temperatures, and it is therefore interesting that the data on two sets of compounds for which this model was particularly successful, namely dichloro-(pyridazine)copper(II) and related complexes and the oxovanadium(IV) carboxylates, included a large proportion of magnetic susceptibilities recorded at temperatures below 100 K.^{6,69,74} Nevertheless, I have already demonstrated that even Bonner and Fisher's own calculations suggest that the low-temperature section of their calculations is suspect. Furthermore, it is in this low-temperature section that experimental susceptibility data are particularly vulnerable to errors due to trace amounts of paramagnetic impurities which would favour a better fit to model (c) than to the others.

My calculation is suspect because of the imperfect choice of the critical-probability criterion [equation (6)], but the predicted susceptibilities agree reasonably well with those of Bonner and Fisher over the common range of up to 11 coupled centres, and the results for chains of length 100 and 101 generate the low-temperature 'dip' which is suggested by Figure 2. My calculation leads to slightly lower susceptibility values than the other two over nearly the whole temperature range. If equation (6a) is used instead the curve is only marginally closer to the others. A detailed inspection of SUP 21938 reveals no pattern in the cases which do favour model (d).

My final conclusions are therefore not decisive, except insofar as I have presented conclusive evidence for the

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rejection of the use of the anisotropic equations obtained from the Ising model for the description of the magnetic properties of these infinite linear-chain systems. I believe that many workers will be disturbed by the fall from grace of the Ising model because of the diminished theoretical basis for the use of magnetic-susceptibility data to support a deduction of a linear-chain structure. It therefore seemed important to attempt to define the limitations of some alternative models. Many may be encouraged by my results to adopt the convenient analytical equation (2) alone, *i.e.* the parallel component of the Ising model, as a basis for such interpretation despite the unsound theoretical foundation for this assumption and the fairly marked divergence from both empirical equations, especially in the region $kT/|J| \simeq 0.5$. Other workers will prefer to use one of the empirical equations, having

noted my reservations about the basis of my calculation and the accuracy of the low-temperature region of the Bonner and Fisher calculation. In general, all of the models fare relatively well for $kT/|J| > 1.0$, but strongly coupled systems and/or low-temperature susceptibility data will require more careful analysis, perhaps through the comparison of several models. Finally, I stress the fact that good empirical data provide scope for checking the validity of any analytical equation obtained in later work.

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