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1996 J. Phys.: Condens. Matter 8 11141

(http://iopscience.iop.org/0953-8984/8/50/037)

J. Phys.: Condens. Matter **8** (1996) 11141–11151. Printed in the UK

The critical temperature and exchange interactions of an $S = 5/2$ Heisenberg antiferromagnet on an f.c.c. lattice

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Received 15 March 1996, in final form 23 August 1996

Abstract. The critical temperature is calculated as a function of the J_{nnn}/J_{nn} ratio for an $S = 5/2$ Heisenberg spin lattice with antiferromagnetic ordering of types I and II on a face-centred cubic lattice. J_{nn} and J_{nnn} represent, respectively, the nearest- and next-nearest-neighbour exchange constants. Both possibilities for ordering of type II, J_{nn} antiferromagnetic and ferromagnetic, are considered. The critical region is studied by applying the Padé approximant method to the corresponding high-temperature series expansion of the staggered susceptibility. The results presented here provide a useful tool for a straightforward interpretation and understanding of experimental data. The approach is applied to various experimental systems and the values obtained compared with those provided by other approximations.

1. Introduction

The face-centred cubic (f.c.c.) lattice is of considerable interest in the theory of antiferromagnetism. This interest arises because of the lack of stability of the ordered structure under only nearest-neighbour (n.n.) interactions. The reason is the inherent 'frustration' that the f.c.c. Heisenberg spin lattice with antiferromagnetic n.n. interactions exhibits—i.e., the inability to simultaneously satisfy all the antiferromagnetic bonds. In fact, such a lattice is one of the basic models of topologically frustrated spin systems. Next-nearest-neighbour (n.n.n.) exchange interactions stabilize the magnetic order on an f.c.c. lattice and have been used by different authors to study the magnetic behaviour of the antiferromagnetic f.c.c. Heisenberg spin lattice [1–3]. From the theoretical point of view the nature of the transition in the f.c.c. Heisenberg antiferromagnet remains less clear. Thus, Diep and Kawamura [4] and Henley [5] have concluded that the transition is first order, in contrast with Fernández *et al* [6], who found a second-order character. No conclusive demonstrations have been given by authors claiming that the transition is first/second order against the results of those claiming the transition to be second/first order. The method we are using here (high-temperature series expansion extrapolated with Padé approximants [7–9]) cannot offer further clarification on this particular point either. Since this method only applies in the paramagnetic zone, the critical region can be approximated only from this zone and not from the ordered zone. From experimental data some f.c.c. compounds have been described to undergo a first-order transition (e.g. UO_2 [10]) while the character of the transition for some others (e.g. CeSe and CeTe [11]) has been reported to be of

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0953-8984/96/5011141+11$19.50

second order. Therefore both first- and second-order kinds of transition have been found experimentally.

Various types of antiferromagnetic ordering arrangement have been described for an f.c.c. lattice. A significant basis for classification of these ordering schemes is one involving the n.n. and n.n.n. spin configurations. Ordering of type I has two-thirds of the n.n. of a reference ion coupled antiferromagnetically while the remainder of the n.n.s as well as all the n.n.n.s are coupled ferromagnetically (see figure 1). In ordering of type II half the n.n.s are antiferromagnetically and half ferromagnetically coupled to the reference ion while all n.n.n.s are coupled antiferromagnetically. Ordering of type III has the same n.n. configuration as ordering of type I, namely two-thirds antiparallel, one-third parallel. However, the n.n.n.s are arranged one-third antiparallel, two-thirds parallel, instead of all parallel as in ordering of type I. In the J_{nnn} versus J_{nn} phase diagram corresponding to these three kinds of ordering, J_{nn} is antiferromagnetic in character for types I and III while it can be antiferromagnetic or ferromagnetic in ordering of the second kind. The exchange constant J_{nnn} is ferromagnetic in character for ordering of type I while antiferromagnetic for type II and III. Moreover type II is stabilized by a comparatively large second- to first-neighbour interaction, generally $|J_{nnn}/J_{nn}| > 0.5$, while ordering of type III requires a smaller ratio, usually $|J_{nnn}/J_{nn}| < 0.5$.

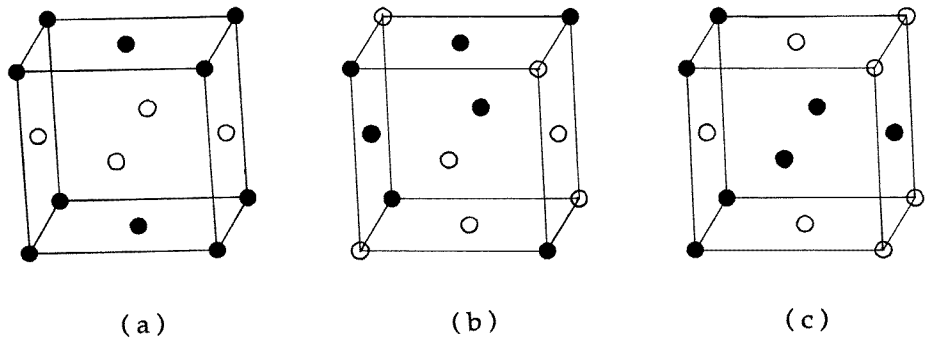

Figure 1. Antiferromagnetic ordering of (a) the first kind, (b) the second kind and (c) the third kind for an f.c.c. lattice. The filled circles represent spins up and the open circles spins down.

The properties of antiferromagnetic ordering on an f.c.c. lattice have been discussed using different theoretical approximations, for example the mean-field method [12], spin-wave theory [5, 13], Green's functions [14–16] and Monte Carlo simulations [1, 4, 6, 17], which have given alternative and independent ways to obtain successive approximations to critical parameters. Unfortunately the limited availability of compounds has resulted in a relatively little experimental work in this field, partially released for $S = 5/2$ [2, 18–20]. However, the recent emergence of novel materials [21–24] opens new opportunities for such studies both to provide the best possible theoretical predictions for comparison with experiments and to pave the way for a better theory.

In this work we shall consider an $S = 5/2$ Heisenberg Hamiltonian with n.n. and n.n.n. interactions, and calculate the critical temperature as a function of the exchange constants for antiferromagnetic ordering on an f.c.c. lattice. The Padé approximant analysis of the exact high-temperature expansions of the magnetic susceptibilities has been shown to be a useful method for the estimation of critical temperatures for real magnetic systems [7]. We shall use this approximation to analyse the critical region. The method considered does

not use as premise the first- or second-order nature of the transition [7–9]. However the mathematical apparatus related to the method uses a continuous function. Therefore the estimation of parameters associated with the critical region (i.e. T_c) would be valid, in a strict consideration, for compounds experiencing a continuous transition. This point should be borne in mind when comparison with experimental data is performed. The predictions for the magnetic exchange constants are expected to be less influenced by the first or second order of the antiferromagnetic transition. On the other hand, the study of the T_c versus J_{nnn}/J_{nn} phase diagram for type II has been usually restricted in the literature to the case of J_{nn} antiferromagnetic [13, 16]. Moreover, the application of the final results of some available theories to the analysis of experimental data requires the knowledge of further parameters [15, 16]. This work intends to provide a valid and straightforward interpretation of experimental data. Comparison with experimental work is also considered.

2. Calculations and results

Although no exact solutions are available in three dimensions for the $S = 5/2$ Heisenberg model with antiferromagnetic ordering on an f.c.c. lattice, it is feasible to obtain exact series expansions for thermodynamic properties in a variable such as $1/T$. The method of exact power-series expansions was extended by Pirnie *et al* to include both n.n. and n.n.n. interactions for the above-mentioned model [25]. The series expansions of the susceptibility in zero magnetic field, $\Psi(K) = \sum a_n K^n$ with $n \geqslant 0$, were derived to the sixth power in reciprocal temperature for types I, II and III. Since we are interested in estimating critical points we have used the Padé approximant (P.A.) method [7–9] to study the dependence of the critical temperature on the relative strength of the first- and second-neighbour interactions. In this work we have used P.A.s as a method of approximate analytic continuation. This method enlarges the convergency radius of the series expansion and may give information on the function in the critical region.

A method of locating an antiferromagnetic singularity uses the series expansion not of the physical susceptibility but of the so-called staggered susceptibility. The advantage of this procedure is that the staggered susceptibility has a strong singularity at the Néel temperature, which may be determined following methods similar to those used for a ferromagnetic singularity. Thus, we have used the high-temperature series expansion in powers of inverse temperature reported above and calculated by Pirnie *et al*. The expression is

$$\{3\chi_s\}/\{|K|X\} = \sum\{a_n(X,\alpha)K^n\}$$

where the summation runs from $n = 0$ to $n = 6$, $X = S(S+1)$, $\chi_s = (\chi^\dagger|J_{nn}|)/(Ng^2\mu_B^2)$, $K = J_{nn}/kT$ and $\alpha = J_{nnn}/J_{nn}$. The staggered susceptibility is represented by $\chi^\dagger$ and the coefficients of the series, which are functions of the X and α parameters, by a_n. For the numerical computation we have considered the f.c.c. lattice with n.n. exchange J_{nn}, n.n.n. exchange J_{nnn}, and all other interactions equal to zero. Throughout this work, we have adopted the convention of taking a general exchange constant, J, positive for ferromagnetic interaction and therefore negative for antiferromagnetic interaction. The Hamiltonian considered is of the type

$$H = -2J_{nn}\sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j - 2J_{nnn}\sum \boldsymbol{S}_k \cdot \boldsymbol{S}_l$$

where the first and second summations run over all pairs of, respectively, nearest and next-nearest neighbours.

The simplest assumption that one can make concerning the nature of the singularity of the magnetic susceptibility is that in the neighbourhood of the critical point the magnetic

susceptibility exhibits an asymptotic behaviour

$$\Psi(K) \approx \{A(K_c - K)^{-\gamma}\}$$

where K_c represents the critical point, γ the critical exponent and A the amplitude. In our case γ is known and equal to 1.43 [26, 27]. Since

$$\{\Psi(K)\}^{1/\gamma} \approx \{A^{1/\gamma}/(K_c - K)\}$$

representations of the series expansions of $\Psi(K)^{1/\gamma}$ by P.A.s would enable us to find K_c by finding the positions of the zeros of the denominator. We have followed this procedure for several values of the first- and second-neighbour exchange constants and ordering of types I, II and III. As a result of these calculations we have obtained the critical temperature T_c as a function of the first- and second-neighbour exchange constants for the f.c.c. $S = 5/2$ Heisenberg model with antiferromagnetic ordering of types I and II. The values are given in table 1. No acceptable convergence was found for type III. This is because several poles were significant and none could be estimated with sufficient accuracy to be able to extract it successfully. More than one pole can be also important in the neighbourhood of a transition between two forms of ordering, as for example takes place for $|J_{nnn}/J_{nn}| \approx 0.5$ on ordering of the second kind.

Table 1. Calculated values of J_{nn}/kT_c as a function of the J_{nnn}/J_{nn} ratio for an $S = 5/2$ Heisenberg model with antiferromagnetic ordering of types I and II on an f.c.c. lattice. (All the values shown in the table are dimensionless). The critical temperature is represented by T_c and the n.n. and n.n.n. exchange constants by, respectively, J_{nn}/k and J_{nnn}/k. (The Hamiltonian to which the exchange constants are referred is of the type $H = -2J_{nn}\sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j - 2J_{nnn}\sum \boldsymbol{S}_k \cdot \boldsymbol{S}_l$)

J_{nnn}/J_{nn}	$(J_{nn}/kT_c)_{type\ I}$	J_{nnn}/J_{nn}	$(J_{nn}/kT_c)_{type\ II}$
−0.01	−0.185	−4.0	0.0102
−0.02	−0.170	−3.6	0.0114
−0.04	−0.146	−3.2	0.0130
−0.06	−0.140	−2.8	0.0149
−0.08	−0.130	−2.4	0.0178
−0.1	−0.124	−2.0	0.0218
−0.2	−0.080	−1.8	0.0247
−0.4	−0.0513	−1.6	0.0288
−0.6	−0.0393	−1.4	0.033
−0.8	−0.0310	−1.2	0.055
−1.0	−0.0263	0.7	−0.103
−1.2	−0.0230	0.8	−0.079
−1.4	−0.0204	1.0	−0.052
−1.6	−0.0183	1.2	−0.040
−1.8	−0.0167	1.4	−0.033
−2.0	−0.0153	1.6	−0.0277
−2.4	−0.0131	1.8	−0.0242
−2.8	−0.0115	2.0	−0.0215
−3.2	−0.0103	2.4	−0.0176
−3.6	−0.0092	2.8	−0.0150
−4.0	−0.0084	3.0	−0.0139
		3.2	−0.0129
		3.6	−0.0114
		4.0	−0.0102

The value of $|J_{nn}/kT_c|$ for type II and $|J_{nnn}/J_{nn}| \gtrsim 1.4$ is independent of the antiferromagnetic or ferromagnetic character of J_{nn}, as reflected in table 1 and figure 2. Below that value, $|J_{nn}/kT_c|$ seems to be not the same for antiferromagnetic or ferromagnetic

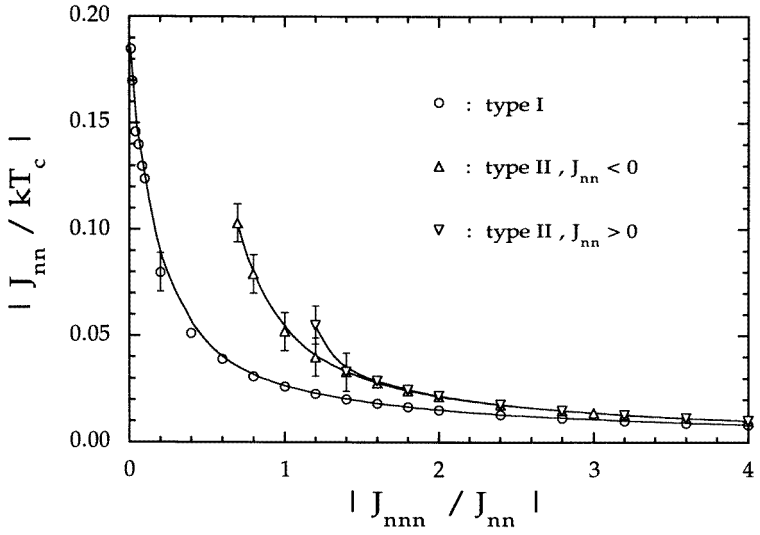

Figure 2. The dependence of $|J_{nn}/kT_c|$ on the $|J_{nnn}/J_{nn}|$ ratio for an $S = 5/2$ Heisenberg model with antiferromagnetic ordering of type I or II on an f.c.c. lattice. The n.n. and n.n.n. exchange constants are represented by, respectively, J_{nn}/k and J_{nnn}/k while T_c represents the critical temperature.

J_{nn}. This result suggests a difference in the behaviour of the system, depending on the sign of J_{nn}. If we consider type II with $J_{nn} < 0$ and the value $|J_{nnn}/J_{nn}|$ is decreased, ordering of type III is reached for $|J_{nnn}/J_{nn}| < 0.5$. The reason is the similarity, regarding exchange constants signs, between type II with $J_{nn} < 0$ and type III. At this point it is worth remarking that $|J_{nnn}/J_{nn}|$ is larger than 0.5 for ordering of the second kind and smaller than that value for ordering of the third kind. On the other hand if type II with $J_{nn} > 0$ is considered and $|J_{nnn}/J_{nn}|$ is decreased below 0.5 then type III ordering can never be reached as happened in the previous case (type II, $J_{nn} < 0$). The reason is that type III requires all the exchange interactions to be antiferromagnetic in character ($J_{nn} < 0, J_{nnn} < 0$) while in the case considered now (type II, $J_{nn} > 0$) the interaction between n.n.s is ferromagnetic. Therefore, the behaviour of the system for small $|J_{nnn}/J_{nn}|$ values is expected not to be the same for $J_{nn} < 0$ and $J_{nn} > 0$. In addition the evolution of $|J_{nn}/kT_c|$ with the ratio $|J_{nnn}/J_{nn}|$ is shown in figure 2 for ordering of the first and second kinds. This figure beautifully illustrates the fact that as J_{nnn} decreases with respect to a reference constant value of J_{nn} the system becomes less stable ($|J_{nn}/kT_c|$ increases).

Up to here we have studied the critical behaviour of an $S = 5/2$ Heisenberg model with antiferromagnetic ordering on an f.c.c. lattice from a high-temperature approximation ($T > T_c$). It would be interesting to compare the results shown in table 1 and figure 2 with an analysis of the critical region from low temperatures, that is $T < T_c$. Lines investigated the antiferromagnetic behaviour in the f.c.c. cubic lattice using a spin-wave method [13]. He devised a method for estimating the critical temperature as a function of the ratio of n.n.n. exchange J_{nnn} to n.n. exchange J_{nn}. The results of both procedures, high-temperature series expansion extrapolated with P.A.s and the spin-wave method from Lines, are depicted together in figure 3 for comparison. Note that the agreement between low- and high-temperature approximations is better/worse for larger/smaller $|kT_c/J_{nn}|$ and $|J_{nnn}/J_{nn}|$ values (a more/less stable system).

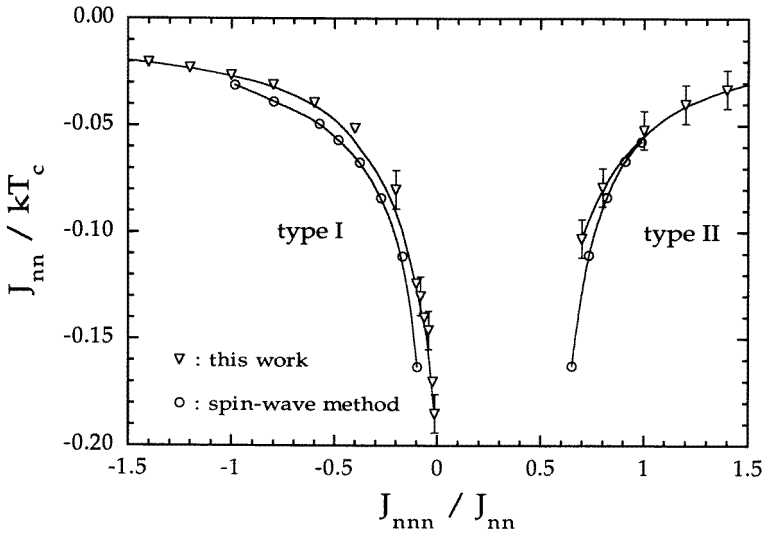

Figure 3. A comparison between a spin-wave method and the results presented in this work for an $S = 5/2$ Heisenberg model with antiferromagnetic ordering of type I or II on an f.c.c. lattice. The n.n. and n.n.n. exchange constants are represented by, respectively, J_{nn}/k and J_{nnn}/k while T_c represents the critical temperature.

The study of the critical temperature versus exchange constants for the Heisenberg model on an $S = 5/2$ f.c.c. lattice with antiferromagnetic ordering of type II has been usually restricted in the literature to the case of J_{nn} antiferromagnetic [13, 16]. On the other hand the application of the final results of some available theories to the analysis of experimental data is not as straightforward as desired. The available approximations, that for the model we consider here give the critical temperature as a function of the exchange constants, require knowledge of the Curie–Weiss constant, θ, of the compound to which the theory is applied [15, 16]. This additional parameter is not required in the work presented here (see table 1 and figure 2). If θ is obtained from experimental data further measurements may be needed, while if it is calculated using the mean-field theory [12] the knowledge of both J_{nn} and J_{nnn} is then required.

3. Comparison with experimental work

Antiferromagnetic behaviour in a f.c.c. lattice has been reported for various compounds, for example K_2ReCl_6 [28, 29], K_2ReBr_6 [28], $MnTe_2$ [30, 31], $[Co(NH_3)_6][FeCl_6]$ [20] or the alloy $MnFeNi_2$ [24] for ordering of type I, CoO [32, 33], MnO [3, 33], NiO [33, 34], α-MnS [2, 35] or the alloy $MnFe_2Ni$ [24] for ordering of type II and β-MnS [36], MnS_2 [31] or K_2IrCl_6 [37, 38] for ordering of type III. In this section the results obtained above are applied to some real f.c.c. $S = 5/2$ systems such as α-MnS, MnO, $MnTe_2$ and $[Co(NH_3)_6][FeCl_6]$. The predictions are expected to reproduce the experimental values depending on the continuous or discontinuous character of the transition. Unfortunately, information about the first- or second-order character of the magnetic transition have only been found in the literature for MnO [39].

The approximation we present in this work is applied in the following to two compounds and the results compared with those obtained by another theoretical method. The random-

phase Green function approximation has been applied to the calculation of superexchange constants in systems such as MnO and α-MnS [16]. In the case of MnO the exchange parameters have also been determined from spin-wave calculations [19, 40, 41]. This low-temperature approximation ($T < T_c$) gives for this compound J_{nn} and J_{nnn} values which are in fair agreement with those deduced from the random-phase Green function approximation [3]. Neutron diffraction experiments suggest that the magnetic structure of both MnO and α-MnS is of type II [33, 35]. We have applied the results shown in table 1 to determine T_c, J_{nnn}/J_{nn} and J_{nnn}/k for these two compounds by using data reported in the literature [2, 3]. The results are presented in table 2. In this table the first line corresponding to α-MnS or MnO contains experimental data for T_c and calculated data for J_{nnn}/J_{nn} and J_{nnn}/k from the random-phase Green function. There is a good agreement in the prediction of the magnetic exchange constants as shown in table 2. The prediction of T_c, which is quite good for α-MnS, shows some differences in the case of MnO ($\sim$7%). In this particular case the discrepancies between experimental and calculated T_c values could be influenced by the first-order character of the transition reported for this compound [39].

Table 2. A comparison with experimental work done on some $S = 5/2$ Heisenberg antiferromagnets with ordering of types I and II. The critical temperature is represented by T_c while J_{nn}/k and J_{nnn}/k represent, respectively, the n.n. and n.n.n. exchange constants. (The Hamiltonian to which the exchange constants are referred is of the type $H = -2J_{nn}\sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j - 2J_{nnn}\sum \boldsymbol{S}_k \cdot \boldsymbol{S}_l$) MFT stands for mean-field theory.

Compound	Ordering	T_c (K)	J_{nnn}/J_{nn}	J_{nnn}/k (K)	Ref.
$MnTe_2$	type I	83	+0.27	−1.6	[30] + MFT
		81	−0.25	+1.5	this work
$[Co(NH_3)_6][FeCl_6]$[a]	type I	0.50	−0.073	+0.005	[20]
		0.51	−0.073	+0.005	this work
α-MnS	type II	147	+1.77	−6.2	[2]
		148	+1.83	−6.4	this work
MnO	type II	117	+1.10	−5.5	[3]
		109	+1.14	−5.7	this work

[a] J_{nn}/k and J_{nnn}/k are calculated respectively from [20] and this work.

In this paragraph the results obtained in section 2 are applied to overcome the problems shown by the mean-field theory regarding the model considered here. Neutron diffraction experiments indicate that $MnTe_2$ orders as an f.c.c. antiferromagnet of type I [31]. Lin and Hacker have calculated the n.n. and n.n.n. exchange constants by applying the mean-field theory to the experimental values $\theta = -472$ K and $T_c = 87.2$ K [30]. Using this approach we have performed a similar calculation but using $T_c = 83$ K instead of $T_c = 87.2$ K. The reason is that the critical temperature associated with the antiferromagnetic ordering of a system corresponds both to the maximum of the peak in the heat capacity measurements, $T_c = 83$ K for $MnTe_2$ [30], and to the value $(\delta\chi/\delta T)_{max}$, where χ represents the magnetic susceptibility. However the maximum in the susceptibility versus temperature curve, $T_c = 87.2$ for $MnTe_2$ [30], is a worse approximation to determine the critical temperature of an antiferromagnetic system [42]. The values we have obtained for the exchange constants are shown in table 2. Although the n.n. interaction is found to be antiferromagnetic in character, mean-field theory indicates that the n.n.n. interaction is also antiferromagnetic, which is in discrepancy with magnetic ordering of type I. The mean-field theory is shown to be far too crude an approximation to give satisfactory quantitative results. Therefore, we have calculated J_{nnn}/k by using the results obtained in section 2 and

the data reported in table 2. Following this procedure a value of $J_{nnn}/k = 1.5$ K is obtained, indicating a ferromagnetic interaction between n.n.n.s, which is in good agreement with the antiferromagnet ordering of type I exhibited by $MnTe_2$.

In the following we present another example of the application of this method to interpret experimental data. Up to here the results presented in this work have been applied to purely inorganic systems. $[Co(NH_3)_6][FeCl_6]$ can be regarded as a close example of a molecular system. Its behaviour would then be of interest in the general area of the recently named 'molecular magnetism' [43, 44]. The magnetic superexchange pathway runs through not only chemical bonds but also softer interactions. Alternating current (a.c.) magnetic susceptibility measurements performed on this compound as a function of the temperature suggest that $[Co(NH_3)_6][FeCl_6]$ orders as an antiferromagnet below 0.5 K. The only magnetic ion present in the compound is Fe(III) since the Co(III) ions are of low spin and therefore have $S = 0$. The n.n. exchange constant $J_{nn}/k = -0.068$ K, has been obtained considering a high-temperature series expansion of the physical susceptibility extrapolated with P.A.s [20]. However, this method was found to be not sensitive enough to changes in the n.n.n. exchange constant. Different J_{nnn} values gave the same fit to the experimental data of $[Co(NH_3)_6][FeCl_6]$. The approximation reported in this work can be used to calculate without ambiguity the n.n.n. exchange constant. A value of $J_{nnn}/k = +0.005 \pm 0.001$ K is obtained by using table 1 and considering an ordering of type I together with the J_{nn} and T_c data reported in the literature. A magnetic ordering of the third kind is unstable since the ratio $|\theta/T_c|$ for $[Co(NH_3)_6][FeCl_6]$, which amounts to 9.2 ($\theta = -4.6$ K for this compound [20]), is smaller than the lower $|\theta/T_c|$ limit of existence of type III [13]. On the other hand, the magnetic superexchange pathways in $[Co(NH_3)_6][FeCl_6]$ are much more favourable between nearest than next-nearest neighbours. Therefore an ordering of the second kind must be also rejected since the corresponding J_{nnn}/J_{nn} ratio is too high ($J_{nnn}/J_{nn} > 0.5$). The critical temperature has been calculated as $T_c = 0.51$ K from J_{nn}, J_{nnn} and the results of section 2. This calculated value is in good agreement with the experimental data, $T_c = 0.50$ K (see table 2).

4. Conclusions

The critical temperature has been calculated as a function of the n.n. and n.n.n. exchange interactions for antiferromagnetic ordering of types I and II and an $S = 5/2$ Heisenberg model on an f.c.c. lattice. Both options for type II, J_{nn} antiferromagnetic and ferromagnetic, are included. High-temperature series expansions extrapolated with Padé approximants are shown to be a convenient method to provide valid estimations of critical temperatures for real magnetic systems. The application of these calculations to some experimental systems and the comparison with other approximations support the validity of the results we have obtained. These theoretical predictions provide a useful tool for a straightforward interpretation and understanding of experimental data. We hope it will be useful for experimental solid state physicists and chemists interested in magnetic properties of materials. Similar studies for smaller spin values are under consideration.

Acknowledgments

The author wishes to thank Professors F Palacio, R Navarro and J F Fernández for a critical reading of the paper and fruitful comments, always with a splendid disposition. This work was supported by the grant No MAT94-0043 from the Comision Interministerial de Ciencia y Tecnología.

Appendix

Coefficients $a_n(X,\alpha)$ of the staggered susceptibility for an f.c.c. lattice and ordering of types I, II and III (from [25]).

A.1. Type I

$$a_0 = 1 \qquad a_1 = -\frac{4}{3}X(2-3\alpha) \qquad a_2 = \frac{2X}{9}\cdot\begin{array}{c|cc} & 1 & X \\ \hline 1 & -10 & +8 \\ \alpha & & -96 \\ \alpha^2 & -9 & +60 \end{array}$$

$$a_3 = \frac{4X}{135}\cdot\begin{array}{c|ccc} & 1 & X & X^2 \\ \hline 1 & +36 & +204 & -176 \\ \alpha & -960 & +720 & \\ \alpha^2 & & +360 & -3840 \\ \alpha^3 & +36 & -486 & +1464 \end{array} \qquad a_4 = \frac{2X}{405}\cdot\begin{array}{c|cccc} & 1 & X & X^2 & X^3 \\ \hline 1 & -126 & +2496 & -448 & -2400 \\ \alpha & & +2256 & +20\,064 & -16\,896 \\ \alpha^2 & & +5304 & -41\,808 & +35\,712 \\ \alpha^3 & & -1152 & +24\,192 & -104\,448 \\ \alpha^4 & -135 & +3060 & -14\,640 & +27\,600 \end{array}$$

$$a_5 = \frac{16X}{42\,525}\cdot\begin{array}{c|ccccc} & 1 & X & X^2 & X^3 & X^4 \\ \hline 1 & +1152 & -42\,276 & -3636 & +108\,792 & -141\,392 \\ \alpha & & -21\,924 & +670\,236 & -73\,248 & -514\,752 \\ \alpha^2 & & -30\,324 & -24\,094 & +2\,482\,032 & -2\,179\,072 \\ \alpha^3 & & -50\,820 & +943\,180 & -3\,287\,760 & +2\,993\,760 \\ \alpha^4 & & +9450 & -303\,030 & +2\,219\,280 & -5\,651\,520 \\ \alpha^5 & +1296 & -38\,961 & +282\,024 & -828\,300 & +1\,128\,360 \end{array}$$

$$a_6 = \frac{2X}{127\,575}\cdot\begin{array}{c|cccccc} & 1 & X & X^2 & X^3 & X^4 & X^5 \\ \hline 1 & -22\,356 & +1\,144\,152 & -8\,973\,444 & +2\,994\,680 & +13\,853\,632 & -15\,163\,392 \\ \alpha & & +395\,280 & -17\,460\,768 & -2\,836\,480 & +61\,894\,656 & -77\,919\,232 \\ \alpha^2 & & +626\,472 & -24\,283\,800 & +169\,210\,608 & -26\,256\,384 & -125\,701\,632 \\ \alpha^3 & & +535\,680 & -5\,024\,160 & -67\,105\,920 & +442\,615\,040 & -394\,024\,960 \\ \alpha^4 & & +1\,030\,248 & -29\,841\,432 & +184\,069\,408 & -432\,265\,728 & +392\,003\,328 \\ \alpha^5 & & -165\,888 & +6\,619\,968 & -71\,298\,432 & +299\,235\,840 & -526\,663\,680 \\ \alpha^6 & -26\,082 & +941\,436 & -9\,367\,506 & +36\,934\,092 & -78\,518\,688 & +83\,019\,648 \end{array}$$

A.2. Type II

$$a_0 = 1 \qquad a_1 = -4X\alpha \qquad a_2 = \frac{2X}{9}\cdot\begin{array}{c|cc} & 1 & X \\ \hline 1 & -12 & -24 \\ \alpha & & \\ \alpha^2 & -3 & +60 \end{array}$$

$$a_3 = \frac{4X}{135}\cdot\begin{array}{c|ccc} & 1 & X & X^2 \\ \hline 1 & +45 & -180 & -480 \\ \alpha & & +360 & +720 \\ \alpha^2 & & & \\ \alpha^3 & +9 & +186 & -1464 \end{array} \qquad a_4 = \frac{2X}{405}\cdot\begin{array}{c|cccc} & 1 & X & X^2 & X^3 \\ \hline 1 & -162 & +4392 & +4560 & -4704 \\ \alpha & & -1152 & -1440 & \\ \alpha^2 & & +2880 & -7632 & -24\,192 \\ \alpha^3 & & & & \\ \alpha^4 & -27 & +36 & -5856 & +27\,600 \end{array}$$

$$a_5 = \frac{16X}{42\,525}\cdot$$

	1	X	X^2	X^3	X^4
1	$+1512$	$-66\,717$	$+227\,913$	$+417\,480$	$-161\,280$
α		$+5859$	$-21\,756$	$-434\,112$	$-809\,088$
α^2		$-21\,105$	$+188\,790$	$-55\,440$	$-766\,080$
α^3		$-17\,640$	$-177\,660$	$+294\,000$	$+1\,058\,400$
α^4					
α^5	$+216$	-2241	$-25\,971$	$+345\,300$	$-1\,128\,360$

$$a_6 = \frac{2X}{127\,575}\cdot$$

	1	X	X^2	X^3	X^4	X^5
1	$-29\,808$	$+1\,746\,576$	$-18\,690\,696$	$+2\,077\,656$	$+36\,640\,128$	$-21\,669\,888$
α		$-60\,912$	$+464\,688$	$+35\,671\,104$	$+8\,042\,496$	$-103\,907\,328$
α^2		$+452\,736$	$-17\,045\,928$	$+18\,005\,904$	$+36\,282\,624$	$-61\,705\,728$
α^3		$+241\,056$	$+905\,184$	$-4\,104\,576$	$-5\,564\,160$	$-5\,160\,960$
α^4		$+292\,464$	$-3\,635\,568$	$+21\,718\,272$	$-10\,453\,248$	$-112\,096\,512$
α^5						
α^6	-3726	$+76\,140$	$+50\,778$	$+4\,618\,572$	$-33\,384\,288$	$+83\,019\,648$

A.3. Type III

$$a_0 = 1 \qquad a_1 = -\frac{4}{3}X(2-\alpha) \qquad a_2 = \frac{2X}{9}\cdot$$

	1	X
1	-10	$+8$
α		-32
α^2	-7	-4

$$a_3 = \frac{4X}{135}\cdot$$

	1	X	X^2
1	$+32$	$+204$	-176
α		-560	-240
α^2		$+280$	
α^3	$+27$	-102	-152

$$a_4 = \frac{2X}{405}\cdot$$

	1	X	X^2	X^3
1	-126	$+2496$	-448	-2400
α		$+1200$	$+7136$	-6144
α^2		$+4440$	$-10\,896$	$-18\,816$
α^3		-864	$+5504$	$+6144$
α^4	-99	$+1380$	$+704$	-1584

$$a_5 = \frac{16X}{42\,525}\cdot$$

	1	X	X^2	X^3	X^4
1	$+1152$	$-42\,276$	-3636	$+108\,792$	$-141\,392$
α		$-13\,293$	$+496\,622$	$+223\,104$	$-588\,224$
α^2		$-25\,704$	$-134\,414$	-4368	$-534\,912$
α^3		$-39\,480$	$+433\,860$	$-78\,960$	$-1\,087\,520$
α^4		$+6930$	$-128\,870$	$-11\,760$	$+190\,400$
α^5	$+936$	$-20\,001$	$+29\,559$	$+60\,180$	-9160

$$a_6 = \frac{2X}{127\,575}\cdot$$

	1	X	X^2	X^3	X^4	X^5
1	$-22\,356$	$+1\,144\,152$	$-8\,953\,668$	$+2\,982\,136$	$+13\,649\,344$	$-15\,407\,104$
α		$+248\,688$	$-12\,189\,312$	$+13\,189\,760$	$+38\,328\,320$	$-67\,963\,904$
α^2		$+537\,696$	$-18\,744\,144$	$+79\,263\,408$	$+71\,439\,872$	$-133\,357\,056$
α^3		$+417\,888$	$-991\,776$	$-20\,403\,712$	$-43\,662\,080$	$-94\,230\,528$
α^4		$+781\,272$	$-17\,295\,864$	$+34\,134\,496$	$+36\,555\,776$	$-74\,670\,336$
α^5		$-119\,808$	$+3\,205\,248$	$-8\,232\,192$	$-12\,577\,280$	$+3\,358\,720$
α^6	$-18\,630$	$+510\,732$	$-2\,472\,846$	$-1\,232\,820$	$+2\,897\,696$	$+102\,272$

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