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M Knežević† and S Milošević‡

† Faculty of Natural Sciences, Kragujevac, Yugoslavia
‡ Institute of Physics, Belgrade, and Department of Physics and Meteorology, Faculty of
Natural and Mathematical Sciences, Belgrade, Yugoslavia

**Abstract.** The compressible Ising chain with the spins $S = 1$ and $S = \frac{3}{2}$ is studied. The lattice and the spin variables are decoupled by using a direct generalisation of the Mattis–Schultz transformation for $S = \frac{1}{2}$. The effective spin Hamiltonian appears to be equivalent to the rigid Ising chain Hamiltonian with an additional biquadratic interaction. We calculate exactly the zero-field free energy, the inital susceptibility and the correlation functions of the effective Hamiltonian. Numerical analysis of the obtained results reveals considerable effects induced by the lattice compressibility.

## 1. Introduction

There has been a latent interest in the influence of the lattice compressiblity on the magnetic behaviour of a one-dimensional Ising system (1D) during the last fifteen years. Mattis and Schultz (1963) were the first to treat the one-dimensional compressible Ising chain. In the appendix of their paper, devoted to a phenomenological theory of the problem, they proved exactly that there is no effect due to the spin–lattice coupling. While Mattis and Schultz (1963) assumed the free-ends boundary conditions and a phonon spectrum corresponding to nearest-neighbour harmonic interactions, Enting (1973) adopted the Einstein phonon spectrum and the periodic boundary conditions. Thus he (Enting 1973) demonstrated that the effective spin Hamiltonian is equivalent to a rigid Ising chain with the nearest and next-nearest neighbour exchange interactions. In the same year, Salinas (1973) proved that the free energy of the 1D compressible Ising chain, whose lattice is exposed to fixed forces, is related to the free energy of the compressible Ising chain, confined to a fixed length, by a standard Legendre transformation. In particular, Salinas (1973) clarified an error in the paper by Bolton and Lee (1970), who overlooked the role of the zero wavevector phonon mode and consequently claimed that the result of Mattis and Schultz (1963) was a by-product of their general treatment of the problem.

Motivated by experiments on the quasi one-dimensional magnets, Mijatović and Milošević (1977) studied a linear Ising chain embedded in a three-dimensional compressible lattice. The perturbative approach of Mijatović and Milošević (1977) was improved by the virtually exact approach of Djordjević and Milošević (1978). The latter authors proved that due to the spin–lattice coupling the magnetic specific heat maximum is reduced and shifted to lower temperatures, whereas a counter-effect was predicted in a simplified treatment of the problem (Oitmaa and Barber 1975). Finally, Figueiredo *et al* (1978) have found exactly the bulk behaviour of a system of the two

compressible Ising chains which are coupled with rigid vertical rods and with exchange interactions along the rods and diagonally between every two rods.

In all previous treatments of the 1D compressible Ising system the conventional two-value ($\pm 1$) spin variables were assumed. Here we present exact results obtained for the 1D compressible Ising model with spin $S = 1$ and $S = \frac{3}{2}$. Using the transfer matrix method we calculated the free energy, the specific heat, the pair correlation functions $\langle S_i S_j \rangle$ and $\langle S_1^2 S_j^2 \rangle$ and the zero-field susceptibility of the corresponding effective spin system. The model and details of the calculations are explained in § 2. Discussion of the obtained results and the appropriate numerical investigations are given in § 3. Links with the treatments of the $S = \frac{1}{2}$ case are established and clarified. It should be noted that, comparing with the work of Mattis and Schultz (1963), we found considerable effects due to the spin–lattice coupling. These effects may be directly ascribed to the induced biquadratic exchange interactions in the effective spin Hamiltonian. Thus our work is also pertinent to the study of the Ising model with the biquadratic exchange, a subject of notable interest in itself (see e.g. Hintermann and Rys 1969, Kinsky and Furman 1975).

## 2. The model and its solution

As we are concerned with effects of the thermal fluctuations of distances between neighbouring spins on the magnetic behaviour of the spin system, we study the following Hamiltonian,

$$\mathcal{H} = J \sum_i S_i S_{i+1} - \gamma \sum_i (x_{i+1} - x_i) S_i S_{i+1} + \frac{1}{2m} \sum_i p_i^2 + \frac{k}{2} \sum_i (x_{i+1} - x_i)^2, \tag{2.1}$$

where $S_i$ is the $z$ projection of the spin at site $i$, $x_i$ is the displacement of site $i$ from its equilibrium position and $\gamma$ is the corresponding first-order change of the exchange function from the rigid-lattice value $J$. The mass and the momentum of the particle at site $i$ are $m$ and $p_i$ respectively, while $k$ is the spring constant between the neighbouring sites. It is assumed that $x_i$ and $p_i$ obey the standard quantum-mechanical commutation relations.

Adopting the free boundary conditions, we can achieve decoupling of the spin and lattice variables in (2.1) by using the unitary transformation

$$U = \prod_n \exp\left(i\frac{\gamma}{k} p_n \sum_{j<n} S_j S_{j+1}\right), \tag{2.2}$$

which is a direct generalisation (Barma 1975) of the transformation used by Mattis and Schultz (1963). In consequence the spin-dependent part of the Hamiltonian (2.1) takes the form

$$\mathcal{H}_{\text{eff}} = J \sum_i S_i S_{i+1} - A \sum_i (S_i S_{i+1})^2, \tag{2.3}$$

with

$$A \equiv \gamma^2/2k, \tag{2.4}$$

where the lattice-dependent part retains the form of the last two sums in (2.1). The appearance of the biquadratic interaction in $\mathcal{H}_{\text{eff}}$ should be observed. If $S_i$ were the two-value variable $S_i = \pm\frac{1}{2}$ (or equivalently $\pm 1$) the corresponding part in $H_{\text{eff}}$ would

result in a constant, and there would be no effect of the spin–lattice coupling (Mattis and Schultz 1963). On the contrary, in the case of spin-1 and spin-$\frac{3}{2}$ ($S_i = 1, 0, -1$ and $S_i = \frac{3}{2}$, $\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$, respectively) there are considerable effects of the biquadratic term in (2.3). In what follows we present results for these two cases. Although the $S = 1$ case appears to be a particular case of a previous study (Krinsky and Furman 1975), we will summarise here our results, not only because they are obtained in a somewhat different way but particularly because they provide a convenient framework for exhibiting the more complex results of the $S = \frac{3}{2}$ case. Thereto we will point out an error in the previous treatment of the problem.

The partition function of the Hamiltonian (2.3) is related to the transfer matrix $\hat{T}$ (Kramers and Wannier 1941) by

$$z_N = \mathrm{Tr}(\hat{T}^N), \tag{2.5}$$

where $N$ is the number of spins in the chain. In the thermodynamic limit ($N \to \infty$) the free energy per spin $F$ can be expressed in terms of the largest eigenvalue $\lambda$ of the transfer matrix,

$$F = -(1/\beta) \ln \lambda, \tag{2.6}$$

where $\beta$ is the reciprocal of the product of the Boltzmann constant $k_B$ and temperature $T$.

In the case $S = 1$ the transfer matrix of (2.3) is of the form

$$\hat{T}_1 = \begin{pmatrix} C & 1 & B \\ 1 & 1 & 1 \\ B & 1 & C \end{pmatrix}, \tag{2.7}$$

where

$$C = \exp[\beta(A - J)] \qquad \text{and} \qquad B = \exp[\beta(A + J)]. \tag{2.8}$$

We found that the transformation $\hat{V}\hat{T}_1\hat{V}^{-1}$ results in a diagonal matrix if $\hat{V}$ and $\hat{V}^{-1}$ are chosen to be

$$\hat{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} a & b & a \\ 1 & 1 & 1 \\ 1 & 0 & -1 \end{pmatrix} \qquad \text{and} \qquad \hat{V}^{-1} = \frac{1}{(a-b)\sqrt{2}} \begin{pmatrix} 1 & -b & a-b \\ -2 & 2a & 0 \\ 1 & -b & b-a \end{pmatrix}, \tag{2.9}$$

with

$$a = (C + B - 1 + K)/2 \qquad \text{and} \qquad b = (C + B - 1 - K)/2, \tag{2.10}$$

and

$$K = [(C + B - 1)^2 + 8]^{1/2}. \tag{2.11}$$

The diagonal elements of the matrix $\hat{V}\hat{T}_1\hat{V}^{-1}$ are

$$\lambda_1 = (C + B + 1 + K)/2, \qquad \lambda_2 = (C + B + 1 - K)/2, \qquad \lambda_3 = C - B, \tag{2.12}$$

where the indices associated with $\lambda$ designate the corresponding row of the matrix.

It can be verified that $\lambda_1$ is the largest diagonal element of $\hat{V}\hat{T}\hat{V}^{-1}$. Hence the free energy per spin of $\mathcal{H}_{\mathrm{eff}}$ is

$$F = -k_B T \ln[(C + B + 1 + K)/2]. \tag{2.13}$$

From expression (2.13) one can easily obtain the magnetic specific heat, but we do not write the rather lengthy formula. The initial susceptibility cannot be obtained from (2.13). For this reason and for the sake of completeness we calculate the two-spin correlation function

$$\langle S_i S_j \rangle_N = \frac{1}{z_N} \sum_{\{S\}} S_i S_j \exp(-\beta \mathcal{H}_{\text{eff}}) = \frac{1}{z_N} \text{Tr}(\hat{T}_1^{N-j+i} \hat{S}_1 \hat{T}_1^{j-i} \hat{S}_1), \tag{2.14}$$

where $i < j$ and the sum is over all possible spin configurations, while $\hat{S}_1$ is the matrix

$$\hat{S}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{2.15}$$

The correlation function (2.14) can be expressed in terms of

$$\tilde{T}_1 = \hat{V} \hat{T}_1 \hat{V}^{-1} \tag{2.16}$$

and

$$\tilde{S} = \hat{V} \hat{S}_1 \hat{V}^{-1}, \tag{2.17}$$

so that

$$\langle S_i S_j \rangle_N = (1/z_N) \text{Tr}(\tilde{T}_1^{N-j+i} \tilde{S}_1 \tilde{T}_1^{j-i-1} \tilde{S}_1), \tag{2.18}$$

or, in the thermodynamic limit,

$$\langle S_i S_j \rangle = \text{Tr} \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tilde{S}_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mu_2^{j-i} & 0 \\ 0 & 0 & \mu_3^{j-i} \end{pmatrix} \tilde{S}_1 \right\}, \tag{2.19}$$

where

$$\mu_2 = \lambda_2/\lambda_1 \qquad \text{and} \qquad \mu_3 = \lambda_3/\lambda_1. \tag{2.20}$$

A simple calculation of the trace in (2.19) yields

$$\langle S_i S_j \rangle = \frac{\lambda_1 - 1}{\lambda_1 - \lambda_2} \mu_3^{j-i}. \tag{2.21}$$

Thus, regardless of the order of $j$ and $i$, we may write

$$\langle S_i S_j \rangle = \frac{\lambda_1 - 1}{\lambda_1 - \lambda_2} \mu_3^{|j-i|}. \tag{2.22}$$

In a quite similar way we find the quadrupolar correlation function

$$\langle S_i^2 S_j^2 \rangle = \left( \frac{\lambda_1 - 1}{\lambda_1 - \lambda_3} \right)^2 - \frac{(\lambda_1 - 1)(\lambda_3 + 1)}{(\lambda_1 - \lambda_3)^2} \mu_2^{|j-i|}. \tag{2.23}$$

By using the fluctuation–dissipation relation (see e.g. Stanley 1971)

$$k_B T \chi_T = \sum_{i,j} \langle S_i S_j \rangle \tag{2.24}$$

we obtain the following expression fo the initial susceptibility per spin:

$$\chi_T = \frac{1}{k_B T} \frac{\lambda_1 - 1}{\lambda_1 - \lambda_2} \frac{\lambda_1 + \lambda_3}{\lambda_1 - \lambda_3}. \tag{2.25}$$

A comparison of formula (2.25) and the corresponding formula in Kinsky and Furman (1975) can reveal a discrepancy between the two. We may attribute it to an error in the derivation of the latter. To this end we checked formula (2.25) by calculating $\chi_T$ in a quite different way from the one exposed here (Suzuki *et al* 1967). We obtained the same result (2.25).

In the case $S = \frac{3}{2}$ the transfer matrix is of the form

$$\hat{T}_{3/2} = \begin{pmatrix} H & M & D & E \\ M & F & G & D \\ D & G & F & M \\ E & D & M & H \end{pmatrix} \tag{2.26}$$

where the matrix elements are

$$H = \exp[9\beta(9A/4 - J)/4], \qquad M = \exp[3\beta(3A/4 - J)/4],$$
$$D = \exp[3\beta(3A/4 + J)/4], \qquad E = \exp[9\beta(9A/4 + J)/4], \tag{2.27}$$
$$F = \exp[\beta(A/4 - J)/4], \qquad G = [\beta(A/4 + J)/4].$$

The transfer matrix (2.26) can be diagonalised by using the matrices

$$\hat{W} = \frac{1}{\sqrt{2}} \begin{pmatrix} R_1 & 1 & 1 & R_1 \\ 1 & R_2 & R_2 & 1 \\ 1 & R_3 & -R_3 & -1 \\ R_4 & 1 & -1 & -R_4 \end{pmatrix}, \qquad \hat{W}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} P_1 & P_2 & L_2 & L_3 \\ P_2 & P_3 & L_1 & L_2 \\ P_2 & P_3 & -L_1 & -L_2 \\ P_1 & P_2 & -L_2 & -L_3 \end{pmatrix} \tag{2.28}$$

where

$$R_1 = \frac{H + E - F - G + K_1}{2(M + D)}, \qquad R_2 = \frac{H + E - F - G - K_1}{2(M + D)},$$

$$R_3 = \frac{E - H + F - G + K_2}{2(M - D)}, \qquad R_4 = \frac{H - E - F + G - K_2}{2(M - D)},$$

$$P_1 = -R_2 P_2, \qquad P_2 = -(R_1 R_2 - 1)^{-1}, \tag{2.29}$$

$$P_3 = -R_1 P_2, \qquad L_1 = -R_4 L_2,$$

$$L_2 = -(R_3 R_4 - 1)^{-1}, \qquad L_3 = -R_3 L_2,$$

with

$$K_1 = [(H + E - F - G)^2 + 4(M + D)^2]^{1/2}, \tag{2.30}$$

and

$$K_2 = [(H - E - F + G)^2 + 4(M - D)^2]^{1/2}. \tag{2.31}$$

The diagonal elements of the matrix $\hat{W}\hat{T}_{3/2}\hat{W}^{-1}$ are

$$\lambda_1' = (H + E + F + G + K_1), \qquad \lambda_2' = \lambda_1' - K_1,$$
$$\lambda_3' = (H - E + F - G + K_2)/2, \qquad \lambda_4' = \lambda_3' - K_2. \tag{2.32}$$

It can be shown that $\lambda_1'$ is the largest diagonal element, and thereby the free energy per spin of the Hamiltonian (2.3), in the case $S = \frac{3}{2}$, has the form

$$F = -k_B T \ln[(H + E + F + G + K_1)/2]. \tag{2.33}$$

From the above expression for $F$ one can straightforwardly derive the magnetic specific heat formula, but we do not quote it here as it is a formidably lengthy formula. On the other hand, the initial susceptibility cannot be obtained from (2.33), and we have to repeat the same steps performed in the $S = 1$ case. Thus, we find the 'dipolar' correlation function

$$\langle S_i S_j \rangle = \tfrac{1}{4}[(L_1 + 3R_1L_2)(3P_1 + R_3P_2)(\lambda_3'/\lambda_1')^{|i-j|}$$
$$+ (L_2 + 3R_1L_3)(3P_1R_4 + P_2)(\lambda_4'/\lambda_1')^{|i-j|}]. \tag{2.34}$$

In addition to $\langle S_i S_j \rangle$ we find the quadrupolar correlation function

$$\langle S_i^2 S_j^2 \rangle = \tfrac{1}{16}[(9R_1P_1 + P_2)^2 + (9P_1 + R_2P_2)(9R_1P_2 + P_4)(\lambda_4'/\lambda_1')^{|i-j|}]. \tag{2.35}$$

The initial susceptibility follows from formulae (2.24) and (2.34):

$$\chi_T = \frac{1}{4k_BT}\Bigg[ (L_1 + 3R_1L_2)(3P_1 + R_3P_2)\frac{\lambda_1' + \lambda_3'}{\lambda_1' - \lambda_3'}$$
$$+ (L_2 + 3R_1L_3)(3P_1R_4 + P_2)\frac{\lambda_1' + \lambda_4'}{\lambda_1' - \lambda_4'}\Bigg]. \tag{2.36}$$

It is a matter of simple algebra to verify that when $A$ goes to zero, i.e. when the lattice compressiblity vanishes, expressions (2.25) and (2.36) reduce to the corresponding expressions obtained for the rigid chains (Suzuki *et al* 1967). Of course the same is true for the magnetic specific heat expressions.

## 3. Discussion

Here we present numerical evaluations of the thermal properties of the effective Hamiltonian (2.3). In figures 1 and 2 we plot the magnetic specific heat for $S = 1$ and
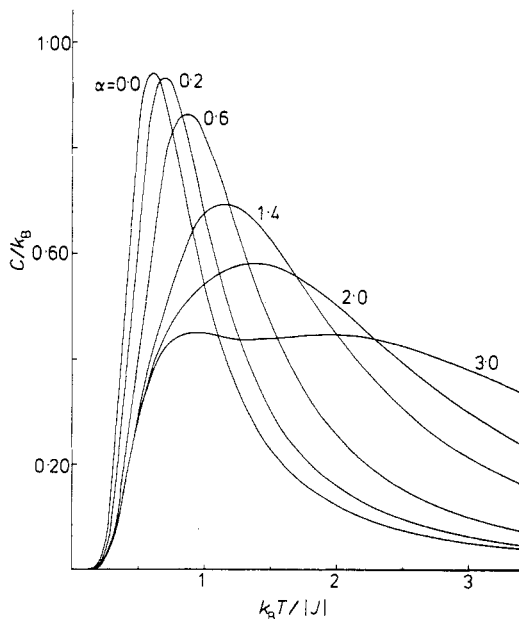


**Figure 1.** The specific heat of the effective Hamiltonian (2.3) with $S = 1$ and for various values of $\alpha = A/J$.
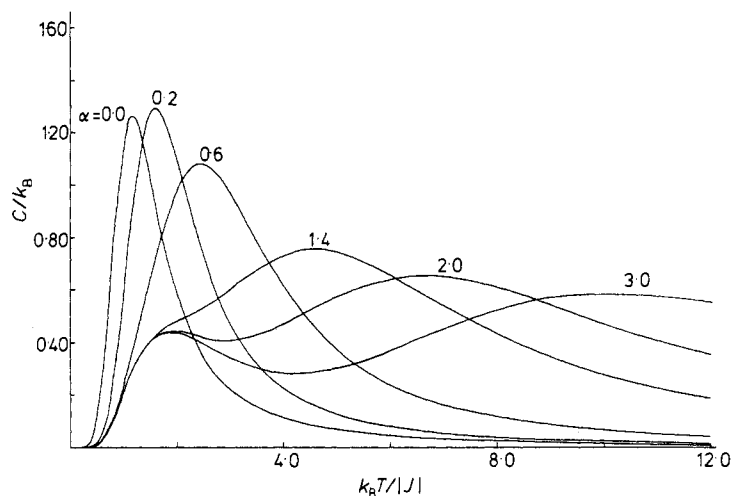
**Figure 2.** The specific heat of the effective Hamiltonian (2.3) with $S = \frac{3}{2}$ and for various values of $\alpha = A/J$.

$S = \frac{3}{2}$ respectively†. We calculated the specific heats for different values of the parameter $\alpha = A/J$, including the rigid chain case $\alpha = 0$. We found that the specific heat is independent of the sign of $\alpha$, which is determined by the sign of $J$ (as $A$ is necessarily a non-negative quantity; see (2.4)). According to the initial form of the Hamiltonian (2.1), $J > 0$ corresponds to the antiferromagnetic case, whereas $J < 0$ corresponds to the ferromagnetic case.
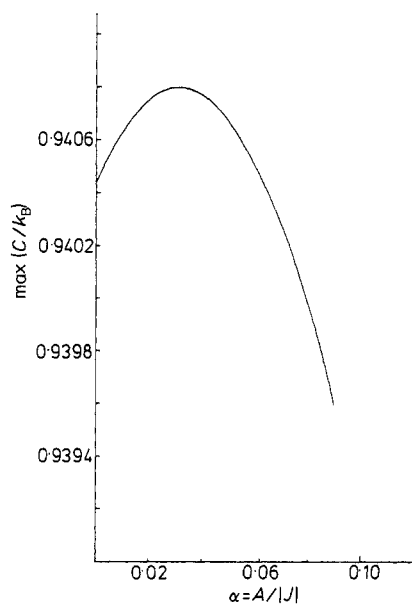


**Figure 3.** The maxima of the specific heats of $H_{\text{eff}}$ for small values of $\alpha = A/J$, in the case $S = 1$.

† Our figure 1 is very similar to figure 1 of Hintermann and Rys (1969). We are grateful to one of the referees for calling our attention to the latter.

From figures 1 and 2 one may notice that a more compressible lattice (i.e. a lower $k$) induces a shift of the specific heat maximum to higher temperatures and a gradual appearance of two broader maxima. These maxima may be attributed to the two different interactions in the effective Hamiltonian (2.3), which bring about short-range orderings associated with the 'magnetic' order parameter $\langle S_i \rangle$ and with the 'quadrupolar' order parameter $\langle S_i^2 \rangle$ (Thorpe and Blume 1972).

In the case $S = \frac{3}{2}$ (see figure 2) it may be observed that the specific heat firstly increases with the increase of the lattice compressibility and afterwards decreases. On the other hand, from figure 1 it could be concluded that in the $S = 1$ case the specific heat maximum always decreases. However, a more detailed calculation (see figure 3) reveals the same behaviour as in the case $S = \frac{3}{2}$. The initial increase of the specific heat maximum, as well as the later appearance of the two broad maxima, is more noticeable in the $S = \frac{3}{2}$ case, for these effects are induced by the biquadratic interaction contribution and it is much larger for $S = \frac{3}{2}$ than for $S = 1$. In figure 4 the $J = 0$ specific heats of the Hamiltonian (2.3) are depicted. One can notice that the biquadratic specific heat is considerably larger for $S = \frac{3}{2}$ than for $S = 1$.
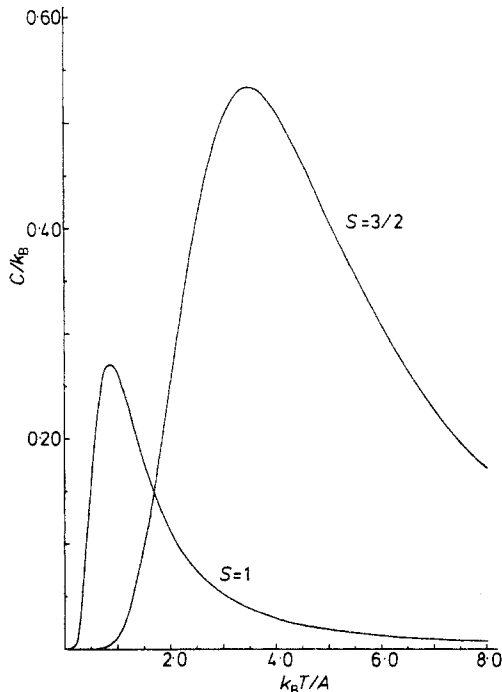


**Figure 4.** The specific heat of the $J = 0$ effective Hamiltonian (2.3).

Concerning the observed shift of the specific heat of the complete Hamiltonian (2.3) to higher temperatures, we may point out that this effect is in agreement with the work of Salinas (1973) and with the result of Djordjević and Milošević (1978). Namely, it follows from Salinas (1973) that a decrease in the lattice rigidity causes a shift of the specific heat to higher temperatures when the fixed-forces boundary conditions are assumed, but it moves the specific heat to lower temperatures in the fixed-volume case. The model studied here corresponds to the case of forces fixed at the zero value.
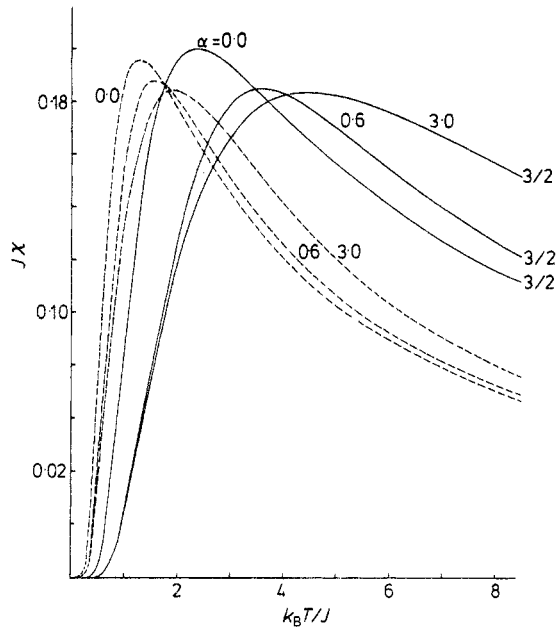
**Figure 5.** The zero-field susceptibility of $H_{eff}$ in the case $J > 0$, for $S = 1$ (the dashed curves) and for $S = \frac{3}{2}$ (the solid curves). Each curve corresponds to a particular value of $\alpha = A/J$.



**Figure 6.** The zero-field susceptibility of $H_{eff}$ in the case $J < 0$, for $S = 1$ (the dashed curves) and for $S = \frac{3}{2}$ (the solid curves). Each curve corresponds to a particular value of $\alpha = A/|J|$.
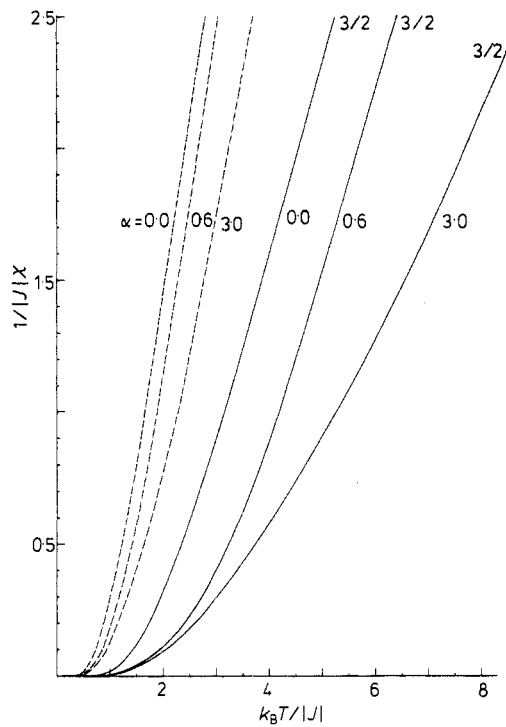
In figures 5 and 6 we plot the zero-field susceptibility of $\mathcal{H}_{\text{eff}}$ for $J > 0$ and $J < 0$ respectively. One should notice that in the antiferromagnetic case $(J > 0)$ the low-temperature slope of the susceptibility decreases with increasing lattice compressiblity, whereas in the ferromagnetic case $(J < 0)$ it is the slope of the reciprocal of the susceptiblity that decreases under the same conditions.

In conclusion, we may state that appreciable effects of the lattice compressiblity on the thermal properties of the Ising chain system with spin $S = 1$, or $S = \frac{3}{2}$, are established. There is no reason in principle why this work could not be extended to the case $S > \frac{3}{2}$. However, one should bear in mind difficulties encountered in the attmpt to obtain, for the $S = 2$ rigid Ising chain (Obokata and Oguchi 1968), the same set of results as those obtained for the rigid $S = 1$ and $S = \frac{3}{2}$ Ising chains (Suzuki *et al* 1967).

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