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TREATMENT OF KINEMATICAL INTERACTION AND ZERO-POINT SPIN REDUCTION IN ANTIFERROMAGNETS

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ABSTRACT

Two kinds of approximation-methods, the metric operator method due to HERBERT and the projection operator method due to ISHIKAWA and OGUCHI, are considered and compared each other. In present paper the former, which has been valid only for $S=1/2$, is extended for general spins. Numerical applications to zero-point spin reduction in real antiferromagnets are performed. It is confirmed that the kinematical interaction plays a decisive role particularly on chain-like substances.

§1. Introduction

Recently, a large zero-point spin reduction has been observed in low dimensional antiferromagnets. In a chain-like antiferromagnet, such as KCuF_3 , the reduction reaches about 50% (DE JONGH and MIEDEMA 1974). It is pointed out by HERBERT (1969) that the kinematical interaction which determines mainly the magnitude of the reduction is not negligible even at absolute zero. For the isotropic Heisenberg antiferromagnet, the free spin wave theory gives the divergent result, since the kinematical interaction is not taken into account properly.

HERBERT (1969) has firstly calculated the reduction for $S=1/2$ by considering the kinematical interaction. ISHIKAWA and OGUCHI (1975: we abbreviate to IO hereafter) have obtained the reduction for general spins in chain-like antiferromagnets and have shown that the contribution from this interaction is really considerably important. HERBERT has used the DYSON-MALEEVE (which is abbreviated to DM) transformation to map the states in the spin space which are orthogonal but not normalized into the orthonormal states in the boson space. The matrix elements in the spin space and in the boson space are connected with each other using a metric operator, which is expressed by a single step function in the case of $S=1/2$. He has investigated the reduction in the ground state of an antiferromagnet with

this metric operator. On the other hand, IO have mapped the orthonormal spin states into the orthonormal boson states, using the HOLSTEIN-PRIMAKOFF (which is abbreviated to HP) transformation. If such a mapping has been done, it is then necessary to introduce a projection operator instead of the metric operator in order to exclude the contributions from the non-physical states which have more spin deviations than $2S+1$.

The metric operator method by HERBERT is extended to general spins and the results obtained are compared with those of IO in the present paper. Further, the application of this method to real chain-like antiferromagnets is considered briefly.

§2. The Boson Mapping

We consider an antiferromagnet which can be divided into two sublattices and take the following Hamiltonian represented by

$$H=2J \sum_{\langle j,m \rangle} \mathbf{S}_j \cdot \mathbf{S}_m - A[\sum_j S_j^z - \sum_m S_m^z], \quad (1)$$

where J is the constant for the antiferromagnetic exchange interaction, and A is the effective anisotropy field in the crystal, and both of them are positive. Subscripts j and m denote the sublattice sites belonging to the up-spin and the down-spin respectively. The summation $\langle j,m \rangle$ must be taken over all nearest neighbor pairs of spins interacting with J .

The state for the j -th atom in the spin space can be represented by

$$|u_j\rangle = [(2S)^{u_j} u_j!]^{-1/2} (S_j^+)^{u_j} |O_j\rangle, \quad (2)$$

where $|O_j\rangle$ is the ground state of the j -th atom. Although these ket vectors $\{|u_j\rangle\}$ are orthogonal with each other, they are not normalized,

$$\langle u_i | v_j \rangle = F_u \delta_{ij} \delta_{uv}, \quad (3)$$

and

$$F_u = 1 \cdot \left(1 - \frac{1}{2S}\right) \cdots \left(1 - \frac{u-1}{2S}\right). \quad (4)$$

The non-physical states whose spin deviations are larger than $2S$ do not appear in the spin space thanks to the factor F_u , and the results obtained in this space should contain no contribution from these non-physical states.

In the boson space, the corresponding state $|u_j\rangle$ can be defined from the ground state $|O_j\rangle$,

$$|u_j\rangle = (u_j!)^{-1/2} (a_j^+)^{u_j} |O_j\rangle. \quad (5)$$

Hereafter we use a_j^+ and a_j , which are creation and annihilation operators for bosons. The vectors $\{|u_j\rangle\}$ are now orthonormal:

$$\langle u_i | v_j \rangle = \delta_{ij} \delta_{uv}. \quad (6)$$

The boson states which have no correspondences in the spin space (the non-physical

states) can exist in this space. In order to exclude the contribution from the non-physical states and to introduce the metric structure as is seen in the spin space, the metric operator η_j is defined as follows (HERBERT 1969, and AKHIEZER et al. 1968),

$$\langle u_j | v_j \rangle = (u_j | \eta_j | v_j) = F_u \delta_{uv}. \quad (7)$$

Here η_j is the Hermitian operator and has an eigenvalue of zero for the non-physical states and non-vanishing values for the physical states. The operators in the spin space can be mapped into the boson space by requiring that all corresponding matrix elements are equal, so that the boson operator \hat{A}_j corresponding to the spin operator A_j is given by

$$\langle u_j | A_j | v_j \rangle = (u_j | \eta_j \hat{A}_j | v_j). \quad (8)$$

The boson operator \hat{A}_j is self-adjoint with respect to the metric operator:

$$\eta_j \hat{A}_j = \hat{A}_j^\dagger \eta_j. \quad (9)$$

However, \hat{A}_j^\dagger does not commute with the metric operator in general,

$$\eta_j \hat{A}_j^\dagger \neq \hat{A}_j^\dagger \eta_j, \quad (10)$$

and, consequently, \hat{A}_j^\dagger is not Hermitian:

$$\hat{A}_j \neq \hat{A}_j^\dagger. \quad (11)$$

It is DM transformation that has the correspondences (7) and (8) and inevitably leads to the undesirable property (11):

$$S_j^\dagger \longrightarrow (2S)^{1/2} (1 - a_j^\dagger a_j / 2S) a_j, \quad S_j^- \longrightarrow (2S)^{1/2} a_j^\dagger,$$

and

$$S_j^z \longrightarrow S - a_j^\dagger a_j. \quad (12)$$

The metric operator for $S=1/2$ is represented by a single step function. DEMBINSKI (1964) obtained an explicit solution of equation (7) for general spins, and another solution may be expressed by a linear combination of unit step functions;

$$\eta_j = \sum_{u=1}^{2S} D_u \theta(u - a_j^\dagger a_j), \quad \theta(x) = \begin{cases} 1, & x \geq 0, \\ 0, & x < 0, \end{cases} \quad (13)$$

$$D_u = F_u - F_{u+1}, \quad \text{and} \quad D_{2S} = F_{2S}, \quad (14)$$

where the coefficients D_u are obtained from equations (7) and (13), and are shown in Table 1.

On the other hand, IO have represented the states in the spin space as follows,

$$|u_j\rangle = [(2S)^{u_j} u_j! F_u]^{-1/2} (S_j^-)^{u_j} |O_j\rangle, \quad u_j \leq 2S. \quad (15)$$

These vectors are now orthonormal and are mapped into the orthonormal boson states (5). Then, IO have introduced the HP transformation, and thus the boson operator \hat{A} has desirably the Hermitian property.

Table 1. Coefficients D_u of the step functions for the metric operator.

S	D_1	D_2	D_3	D_4	D_5
$\frac{1}{2}$	1				
1	$\frac{1}{2}$	$\frac{1}{2}$			
3	$\frac{1}{3}$	$\frac{4}{9}$	$\frac{2}{9}$		
2	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{9}{32}$	$\frac{3}{32}$	
$\frac{5}{2}$	$\frac{1}{5}$	$\frac{8}{25}$	$\frac{36}{125}$	$\frac{96}{625}$	$\frac{24}{625}$

$$S_j^+ \longrightarrow (2S)^{1/2}(1 - a_j^\dagger a_j / 2S)^{1/2} a_j, \quad S_j^- \longrightarrow (2S)^{1/2} a_j^\dagger (1 - a_j^\dagger a_j / 2S)^{1/2},$$

and

$$S_j^z \longrightarrow S - a_j^\dagger a_j. \quad (16)$$

However, the representation (16) should be restricted to the boson-state where the boson occupation number is smaller than $2S+1$. It is, therefore, necessary to introduce a projection operator P_j ,

$$P_j = \theta(2S - a_j^\dagger a_j), \quad (17)$$

where $\theta(x)$ is a unit step function defined as in equation (13).

The relation between the DM and the HP transformation has been discussed fully in terms of the metric operator by DEMBINSKI (1964) and HERBERT (1969).

§3. Zero-Point Spin Reduction

We introduce the DM transformation into the Hamiltonian (1):

$$\begin{aligned} S_j^+ &\longrightarrow (2S)^{1/2}(1 - a_j^\dagger a_j / 2S) a_j, & S_m^+ &\longrightarrow (2S)^{1/2} b_m^+, \\ S_j^- &\longrightarrow (2S)^{1/2} a_j^\dagger, & S_m^- &\longrightarrow (2S)^{1/2}(1 - b_m^\dagger b_m / 2S) b_m, \\ S_j^z &\longrightarrow S - a_j^\dagger a_j, & \text{and} & \\ S_m^z &\longrightarrow -S + b_m^\dagger b_m. \end{aligned} \quad (18)$$

Further, the Fourier- and the Bogoliubov-transformation are introduced to obtain the diagonalized harmonic Hamiltonian:

$$a_j = N^{-1/2} \sum_k \exp(i\mathbf{k} \cdot \mathbf{R}_j) a_k, \quad b_m = N^{-1/2} \sum_k \exp(-i\mathbf{k} \cdot \mathbf{R}_m) b_k, \quad (19)$$

$$\alpha_k = u_k a_k - v_k b_k^\dagger, \quad \text{and} \quad \beta_k = u_k b_k - v_k a_k^\dagger. \quad (20)$$

Then the excitation energy of a spin wave is given by

$$\lambda_k = 2JSZ\sqrt{(1+A/2JSZ)^2 - \gamma_k^2}, \quad (21)$$

where

$$\gamma_k = Z^{-1} \sum_{\delta} \exp(\mathbf{i}\mathbf{k} \cdot \boldsymbol{\delta}),$$

$$u_k = \pm [2JSZ(1+A/2JSZ) + \lambda_k]^{1/2},$$

and

$$v_k = \mp [2JSZ(1+A/2JSZ) - \lambda_k]^{1/2}. \quad (22)$$

Here $\boldsymbol{\delta}$ denotes the vectors from a given atom to the Z nearest neighbors interacting with the strength J . When the HP transformation is introduced into the Hamiltonian (1) instead of the DM transformation (18);

$$\begin{aligned} S_j^+ &\longrightarrow \langle 2S \rangle^{1/2} (1 - a_j^+ a_j / 2S)^{1/2} a_j, & S_m^- &\longrightarrow \langle 2S \rangle^{1/2} b_m^+ (1 - b_m^+ b_m / 2S)^{1/2}, \\ S_j^- &\longrightarrow \langle 2S \rangle^{1/2} a_j^+ (1 - a_j^+ a_j / 2S)^{1/2}, & S_m^- &\longrightarrow \langle 2S \rangle^{1/2} (1 - b_m^+ b_m / 2S)^{1/2} b_m, \\ S_j^z &\longrightarrow S - a_j^+ a_j, & \text{and} & & S_m^z &\longrightarrow -S + b_m^+ b_m, \end{aligned} \quad (23)$$

we obtain the spectrum (21) again by a similar way.

The expectation value of S^z for a spin in each sublattice is expressed by the relation $\langle S_j^z \rangle = S - \Delta S$, where ΔS is the zero-point spin reduction given by equations (8) and (18);

$$\frac{\langle \tilde{O} | \eta a^+ a | \tilde{O} \rangle}{\langle \tilde{O} | \eta | \tilde{O} \rangle} = \frac{\langle \tilde{O} | S - S^z | \tilde{O} \rangle}{\langle \tilde{O} | \tilde{O} \rangle} = \Delta S. \quad (24)$$

Here $|\tilde{O}\rangle$ is the exact ground state in the boson space and $|\tilde{O}\rangle$ is the corresponding one in the spin space. In IO's treatment, the projection operator P is introduced into equation (24) instead of η .

The metric operator η is a product of the metric operators of all lattice sites, that is, $\eta = \prod_j \eta_j$, and the following approximation is introduced in the real calculation:

$$\frac{\langle \tilde{O} | \eta a_j^+ a_j | \tilde{O} \rangle}{\langle \tilde{O} | \eta | \tilde{O} \rangle} \simeq \frac{\langle \tilde{O} | \eta_j a_j^+ a_j | \tilde{O} \rangle}{\langle \tilde{O} | \eta_j | \tilde{O} \rangle}. \quad (25)$$

TAO YUIN (1966) has given the expansion formula of a step-function:

$$\theta(u - a_j^+ a_j) = \sum_{n=0}^{\infty} B_n (a_j^+)^n (a_j)^n,$$

and

$$a_j^+ a_j \theta(u - a_j^+ a_j) = \sum_{n=1}^{\infty} C_n (a_j^+)^n (a_j)^n, \quad (26)$$

where

$$\begin{aligned} B_0 &= 1, & B_n &= 0, & n &\leq u, \\ B_n &= \frac{(-1)^{n-u} (u+1)(u+2)\cdots(n-1)}{n! (n-u-1)!}, & n &\geq u+1, \\ C_1 &= 1, & C_n &= 0, & n &\leq u, \end{aligned}$$

and

$$C_n = \frac{(-1)^{n-u} u(u+1) \cdots (n-2)}{(n-1)! (n-u-1)!}, \quad n \geq u+1. \quad (27)$$

The true ground state $|\tilde{O}\rangle$ is approximated by the magnon ground state $|\hat{O}\rangle$ in the free spin wave theory. Then we obtain

$$(\hat{O}|\alpha_j^n)(\alpha_j^n|\hat{O}) = n! V^n, \quad (28)$$

where

$$V = N^{-1} \sum_k v_k^2. \quad (29)$$

Here v_k is the coefficient which appears in the Bogoliubov transformation (20), and V is the spin reduction in the free spin wave theory. From equations (13), (14), (17) and (24), the reduction $\mathcal{A}S$ for a general spin is obtained for the both cases:

$$\mathcal{A}S_M = V - \frac{\sum_{u=1}^{2S} D_u (1+u) (1+V)^{-(1+u)} V^{1-u}}{\sum_{u=1}^{2S} D_u (1+V)^{-(1+u)} V^{1+u}}, \quad \text{the metric operator method,} \quad (30)$$

and

$$\mathcal{A}S_P = V - \frac{(2S+1)V^{2S+1}}{(1+V)^{2S+1} - V^{2S+1}}, \quad \text{the projection operator method.} \quad (31)$$

Table 2. The limiting values of zero-point spin reduction where the anisotropy field A tends to zero.

Square lattice		
S	$\mathcal{A}S_P$	$\mathcal{A}S_M$
1/2	0.141	0.141
1	0.184	0.163
3/2	0.194	0.172
2	0.197	0.177
5/2	0.197	0.181
free spin wave theory	0.197	
NaCl-type lattice		
S	$\mathcal{A}S_P$	$\mathcal{A}S_M$
1/2	0.067	0.067
1	0.077	0.072
3/2	0.078	0.074
2	0.078	0.075
5/2	0.078	0.076
free spin wave theory	0.078	

Using the formulae (30) and (31), we have carried out the numerical calculations for the spin reduction of the case with non-vanishing A as well as the case with vanishing A as the limiting case. The values of ΔS for two and three dimensional systems with $A=0$ are shown in Table 2 together with those of IO. As for the non-vanishing A , the values obtained for one, two and three dimensions and for different S values are shown in Table 3. We have shown the spin reduction of

Table 3. Zero-point spin reduction for various spin values: (a) one dimension, (b) two dimension (square lattice) and (c) three dimension (NaCl-type lattice). The values of ΔS_M and ΔS_P are given by expressions (30) and (31) respectively.

(a) one dimensional system

	S=1/2		S=1		S=3/2		S=2		S=5/2	
$A/2J$	ΔS_M	ΔS_P								
1×10^{-1}	0.162	0.162	0.242	0.285	0.299	0.364	0.342	0.419	0.376	0.459
4×10^{-2}	0.211	0.211	0.305	0.366	0.370	0.469	0.420	0.539	0.459	0.588
1×10^{-2}	0.266	0.266	0.382	0.466	0.460	0.605	0.519	0.702	0.566	0.771
4×10^{-3}	0.294	0.294	0.422	0.519	0.508	0.681	0.574	0.798	0.627	0.881
1×10^{-3}	0.325	0.325	0.470	0.582	0.568	0.777	0.643	0.922	0.705	1.030
4×10^{-4}	0.342	0.342	0.496	0.616	0.601	0.830	0.683	0.993	0.749	1.117
1×10^{-4}	0.361	0.361	0.528	0.658	0.644	0.898	0.733	1.086	0.808	1.236

(b) two dimensional system

	S=1/2		S=1		S=3/2		S=2		S=5/2	
$A/2J$	ΔS_M	ΔS_P								
1×10^{-1}	0.094	0.094	0.119	0.130	0.131	0.144	0.140	0.151	0.146	0.156
4×10^{-2}	0.113	0.113	0.137	0.152	0.148	0.164	0.155	0.169	0.160	0.173
1×10^{-2}	0.125	0.125	0.148	0.165	0.158	0.177	0.165	0.180	0.169	0.183
4×10^{-3}	0.132	0.132	0.154	0.173	0.164	0.184	0.170	0.187	0.174	0.189
1×10^{-3}	0.136	0.136	0.158	0.177	0.167	0.188	0.173	0.190	0.177	0.192
4×10^{-4}	0.138	0.138	0.160	0.180	0.169	0.191	0.175	0.193	0.178	0.194
1×10^{-4}	0.140	0.140	0.161	0.182	0.171	0.192	0.176	0.194	0.179	0.195

(c) three dimensional system

	S=1/2		S=1		S=3/2	
$A/2J$	ΔS_M	ΔS_P	ΔS_M	ΔS_P	ΔS_M	ΔS_P
1×10^{-1}	0.057	0.057	0.065	0.069	0.069	0.072
4×10^{-2}	0.063	0.063	0.070	0.074	0.072	0.076
1×10^{-2}	0.066	0.066	0.071	0.076	0.073	0.078
4×10^{-3}	0.067	0.067	0.072	0.077	0.074	0.078
1×10^{-3}	0.067	0.067	0.072	0.077	0.074	0.078
4×10^{-4}	0.068	0.068	0.072	0.077	0.074	0.078
1×10^{-4}	0.068	0.068	0.072	0.077	0.074	0.078

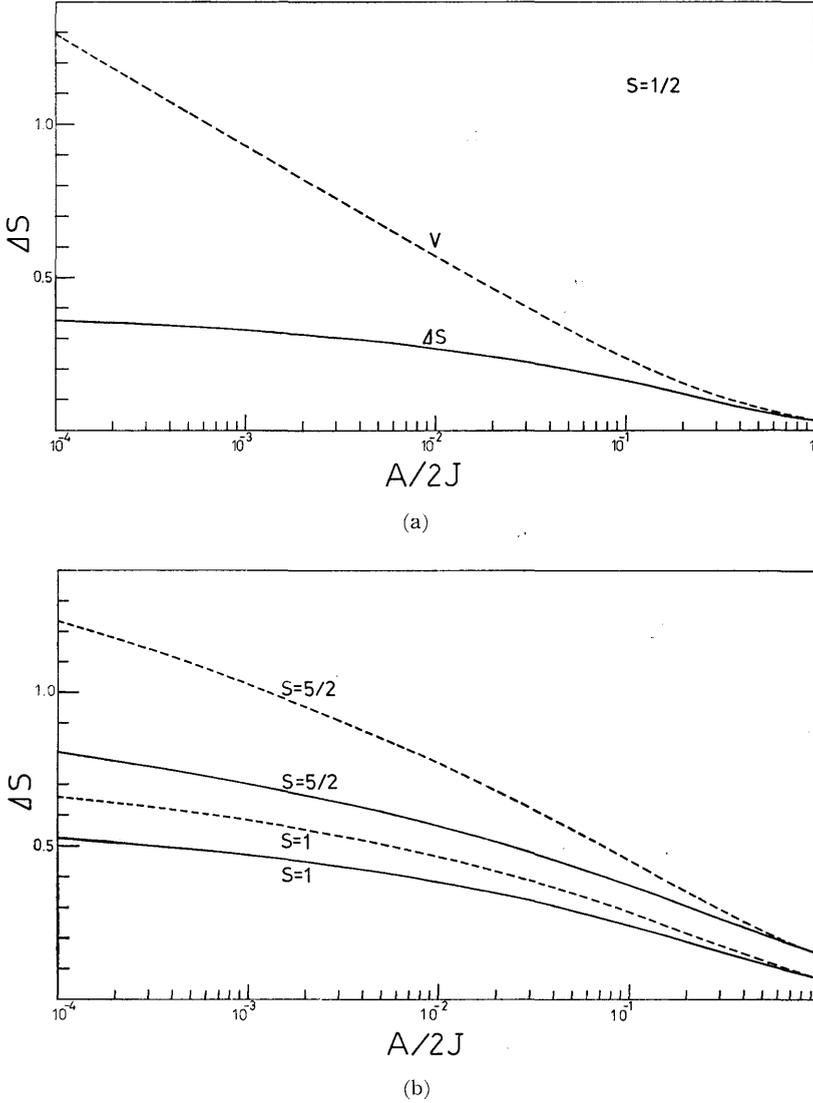


Fig. 1. Zero-point spin reduction of one dimensional system. (a) The solid line and the broken line correspond to ΔS and V respectively. (b) Solid lines: ΔS_M given by equation (30). Broken lines: ΔS_P given by (31).

the one dimensional system for $S=1/2$ in Fig. 1 (a), and for $S=1$ and $5/2$ in Fig. 1 (b). Fig. 1(a) shows the spin reduction ΔS (the solid line) and the spin reduction V in the free spin wave theory (the broken line) for $S=1/2$. Since $S=1/2$, equations (30) and (31) give the same results. Fig. 1 (b) shows the spin reduction ΔS_M (the solid lines) given by equation (30) and the spin reduction ΔS_P (the broken lines) by equation (31). It is seen that the kinematical interaction is contributing considerably in this system.

Though the spin reduction tends to infinity for an isotropic one dimensional system in the free spin wave theory, the values of ΔS tend to S in the present theory when the anisotropy field A approaches to zero, since the kinematical interaction is taken into account properly. The ratio of ΔS to the magnitude of S becomes larger as the dimensionality becomes lower, or as the spin value S becomes smaller as is clearly seen in Table 3.

§4. Discussion

A large spin reduction ($\sim 50\%$) has been observed in the so-called one dimensional antiferromagnet such as KCuF_3 . In this substance, it is found that the antiferromagnetic order is developed along the c -axis, and there are weak ferromagnetic interactions between chains. It may be considered that the weak interactions between chains in the chain-like antiferromagnet can be replaced by the effective anisotropy field in one dimensional system.

In order to investigate this idea, we take the following Hamiltonian:

$$H = 2J \sum_{\langle j,l \rangle} \mathbf{S}_j \cdot \mathbf{S}_l - 2J' \sum_{\langle m,n \rangle} \mathbf{S}_m \cdot \mathbf{S}_n, \quad (32)$$

and have carried out numerical calculations to it, where J denotes the exchange interaction between spins which belong to two different sublattices in a chain, and J' denotes the ferromagnetic interaction between different chains. Following the procedure described in §3, we may obtain the diagonalized Hamiltonian as follows:

$$\begin{aligned} H &= E_0 + \sum_k \lambda_k (\alpha_k^+ \alpha_k + \beta_k^+ \beta_k), \\ E_0 &= -2JNS^2 Z(1 + \zeta\nu) + \sum_k \{\lambda_k - 2JSZ(1 + \zeta\nu)\}, \\ \lambda_k &= 2JSZ \sqrt{\{1 + \zeta\nu(1 - \gamma_k')\}^2 - \gamma_k^2}, \\ \gamma_k &= Z^{-1} \sum_q \exp(i\mathbf{k} \cdot \boldsymbol{\delta}), \quad \gamma_k' = Z'^{-1} \sum_q \exp(i\mathbf{k} \cdot \boldsymbol{\delta}'), \\ \zeta &= J'/J, \quad \text{and} \quad \nu = Z'/Z. \end{aligned} \quad (33)$$

The vectors $\boldsymbol{\delta}$ and $\boldsymbol{\delta}'$ denote the vectors from a given atom to the Z and Z' nearest neighbors, which interact through J and J' respectively. We have computed the spin reduction of the chain-like antiferromagnet for $S=1/2$ as well as for $S=1$ and $5/2$. Fig. 2 (a) shows the spin reduction ΔS (the solid line) and the reduction V in the usual free spin wave theory (the broken line) for $S=1/2$. In Fig. 2 (b), the solid lines and the broken lines correspond to the spin reduction ΔS_M given by equation (30) and the reduction ΔS_P by equation (31) for $S=1$ and $5/2$, respectively.

Fig. 1 corresponds with the case where the antiferromagnetic order arises from the staggered field A for one dimensional antiferromagnet. Fig. 2 corresponds to that from the ferromagnetic interaction J' between the antiferromagnetic chains. We may connect these two results and obtain the relation between A and J' . If we replace these interchain interaction by the effective staggered fields for

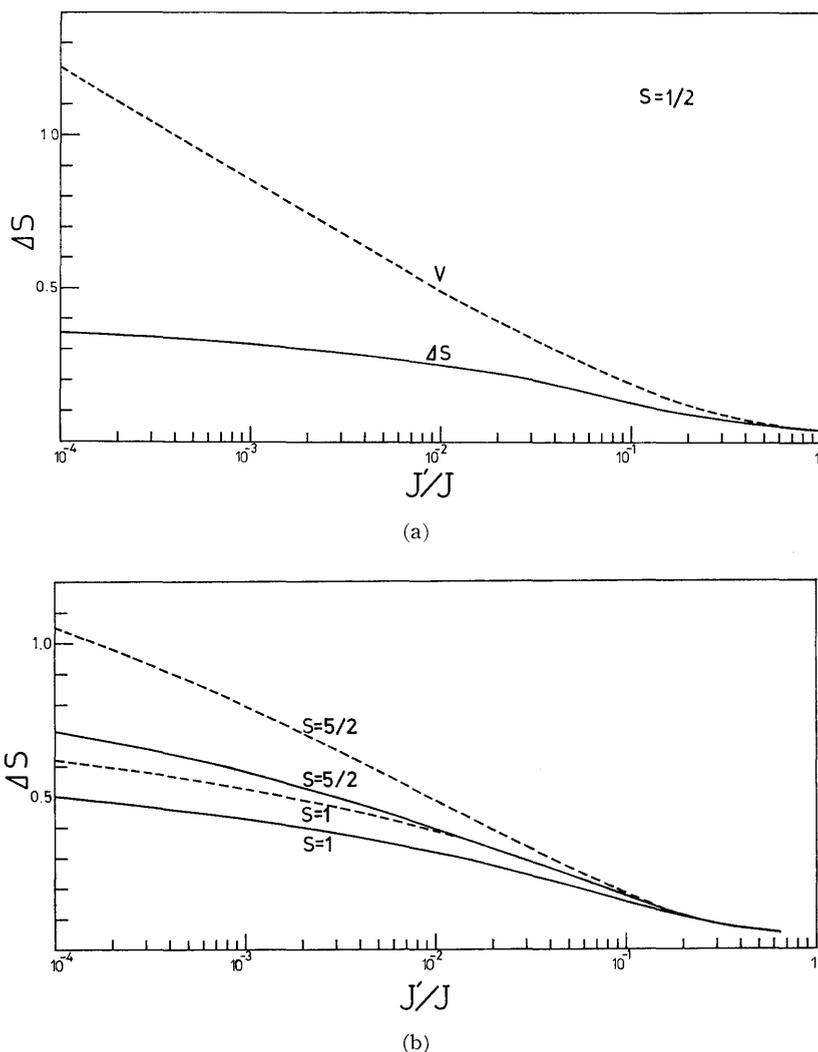


Fig. 2. Zero-point spin reduction of a chain-like antiferromagnet. (a) Solid line: the values of ΔS . Broken line: the values of V . (b) Solid lines: ΔS_M given by equation (30). Broken lines: ΔS_P given by (31).

the z -direction, it may be expected that the relation $A=2J'Z'\langle S^z \rangle$ would hold on the simple molecular-field-theoretical point of view. However, it seems that we should prefer the relation $A=2J(Z'-1)S$ numerically from these results obtained above.

From the discussion mentioned above, we may apply the theory to other materials with $S > 1/2$ as well as KCuF_3 , $\text{CuCl}_2 \cdot 2\text{NC}_5\text{H}_5$ and $\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$ with $S=1/2$. The zero-point spin reductions ΔS obtained for these chain-like substances are shown in Table 4, using the Hamiltonian (32) where we have used the values for $\zeta (=J'/J)$ given by DE JONGH and MIEDEMA (1974).

Table 4. Zero-point spin reduction of real chain-like antiferromagnets.

	S	J'/J	ΔS_M	ΔS_P
KCuF ₃	1/2	2.7×10^{-2}	0.21 (42%)	0.21 (42%)
CuCl ₂ ·2NC ₅ H ₅	1/2	4×10^{-3}	0.28 (56%)	0.28 (56%)
Cu(NH ₃) ₄ SO ₄ ·H ₂ O	1/2	6×10^{-3}	0.27 (54%)	0.27 (54%)
CrCl ₂	2	5×10^{-2}	0.24 (12%)	0.27 (13%)
CsMnCl ₃ ·2H ₂ O	5/2	6×10^{-3}	0.45 (18%)	0.56 (22%)

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