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KINEMATICAL AND DYNAMICAL INTERACTION IN CHAIN-LIKE ANTIFERROMAGNETS

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ABSTRACT

The contributions of kinematical and dynamical interaction to zero-point spin reduction of a chain-like antiferromagnet are investigated. Kinematical interaction is considered by two methods, the metric operator method and the projection operator method. The biquadratic terms of boson operators are treated self-consistently with the idea of mean fields to include the effects of dynamical interaction. The case of ferromagnetic inter-chain exchange interaction as well as the case of antiferromagnetic inter-chain interaction are considered and the results obtained are compared with each other.

§ 1. Introduction

In a previous paper (FUKUCHI and OKABE 1977), the metric operator method by HERBERT (1969) was developed to get the zero-point spin reduction of antiferromagnets for general spins and the results obtained have been compared with those of the projection operator method by ISHIKAWA and OGUCHI (1975, hereafter we abbreviate it as IO). The usual free spin wave theory which contains the contribution from the fictitious non-physical boson states gives the divergent reduction in the isotropic one-dimensional Heisenberg system. When the kinematical interaction is taken into account properly, the reduction reaches at most up to the order of magnitude of S even in the isotropic case. The value of the reduction goes to S when the effective anisotropy field A or the inter-chain exchange interaction J' goes to zero. A large contribution coming from non-physical states is found in the ideal one-dimensional system, and also in the real chain-like antiferromagnets with non-vanishing A and J'.

On the contrary, the isotropic two- and three-dimensional Heisenberg systems have the non-divergent reductions even in the usual free spin wave theory. Even if the kinematical interaction is considered, the reductions are found to decrease slightly in their magnitude. Thus, the effect of the kinematical interaction is small but, as we should notice, not negligible for these systems.

In the present paper, we consider the spin-reduction of the chain-like antiferromagnets with the metric oprator method as well as the projection operator method. HERBERT (1969) has used the former in order to exclude the contribution arising from non-physical states and introduced the Dyson-Maleev (hereafter it is abbreviated to DM) transformation to rewrite the Hamiltonian described by spin operators into boson operators. On the other hand, IO have normalized the states in the spin space and introduced the projection operator using the Holstein-Primakoff (hereafter it is abbreviated to HP) transformation.

It is known that long range order in the chain-like antiferromagnet, such as $KCuF_3$, is caused due to the inter-chain exchange interaction (IKEDA and HIRAKAWA 1973). This inter-chain interaction in $KCuF_3$ is found to be ferromagnetic. We investigate the case of the weak ferromagnetic inter-chain interaction at first in the harmonic approximation and then we treat the case of the antiferromagnetic inter-chain interaction. In order to compare the contribution arising from kinematical interaction with that from dynamical interaction, the biquadratic terms of boson operators are self-consistently dealt with using the idea of mean fields. The effect of the dynamical interaction is found to be small and the large zero-point spin reduction can be attributed mainly to the kinematical interaction.

§ 2. Treatment of Kinematical Interaction in the Harmonic Approximation

We consider the Hamiltonian for the chain-like antiferromagnet with the ferromagnetic inter-chain interaction:

$$H=2J\sum_{j,l}\boldsymbol{S}_j\cdot\boldsymbol{S}_l-2J'\sum_{<m,n}\boldsymbol{S}_m\cdot\boldsymbol{S}_n\,, \tag{1}$$

where J and J' are the intra-chain and the inter-chain exchange interactions respectively, and both of them are positive. Subscripts j and l denote up-spin and down-spin sublattice sites respectively, and pairs of m and n represent sites in the identical sublattice. The summations over $\langle j,l\rangle$ and $\langle m,n\rangle$ are taken over all nearest neighbor pairs of spins interacting with J and J', respectively.

The DM transformation is introduced into the Hamiltonian (1):

$$\begin{aligned}
&S_j^{+}\to\sqrt{2S}(1-a_j^{+}a_j/2S)a_j, &&S_l^{+}\to\sqrt{2S}b_l^{+}\,,\\
&S_j^{-}\to\sqrt{2S}a_j^{+}\,, &&S_l^{-}\to\sqrt{2S}(1-b_l^{+}b_l/2S)b_l,\\
&S_j^{z}\to S-a_j^{+}a_j,\ \text{and} &&S_l^{z}\to -S+b_l^{+}b_l.
\end{aligned}\tag{2}$$

The boson operators are Fourier-transformed in the usual way:

$$a_j=N^{-1/2}\sum_k \exp(i\boldsymbol{k}\cdot\boldsymbol{R}_j)a_k, \text{ and } b_l=N^{-1/2}\sum_k \exp(-i\boldsymbol{k}\cdot\boldsymbol{R}_l)b_k, \tag{3}$$

then we get the following Hamiltonian:

$$H_{\mathrm{DM}}=-2JNZS^2(1+\zeta\nu)+2JSZ\sum_k[\{1+\zeta\nu(1-\gamma_k')\}(a_k^+a_k+b_k^+b_k)$$
$$+\gamma_k(a_kb_k+a_k^+b_k^+)]-2JZN^{-1}\sum_{k1,k2,k3}[\gamma_{k1-k2}a_{k1}^+a_{k2}b_{k3}^+b_{-k1+k2+k3}$$
$$+\frac{1}{2}(\gamma_{-k1+k2-k3}a_{k1}^+a_{k2}a_{k3}b_{-k1+k2+k3}+\gamma_{k1}a_{k1}b_{k2}^+b_{k3}b_{k1+k2-k3})], \tag{4}$$

where

$$\gamma_k=Z^{-1}\sum_\delta \exp(i\boldsymbol{k}\cdot\boldsymbol{\delta}), \qquad \gamma_k'=Z'^{-1}\sum_{\delta'}\exp(i\boldsymbol{k}\cdot\boldsymbol{\delta}'),$$
$$\zeta=J'/J, \text{ and } \qquad \nu=Z'/Z. \tag{5}$$

Here, as we are interested in the region $J'\ll J$, only the biquadratic terms with J are treated.

On the other hand, if the HP transformation is put into Hamiltonian (1),

$$S_j^+\to\sqrt{2S}(1-a_j^+a_j/2S)^{1/2}a_j, \qquad S_l^+\to\sqrt{2S}\,b_l^+(1-b_l^+b_l/2S)^{1/2},$$
$$S_j^-\to\sqrt{2S}a_j^+(1-a_j^+a_j/2S)^{1/2}, \qquad S_l^-\to\sqrt{2S}(1-b_l^+b_l/2S)^{1/2}b_l,$$
$$S_j^z\to S-a_j^+a_j, \text{ and } \qquad S_l^z\to -S+b_l^+b_l, \tag{6}$$

we obtain the following Hamiltonian in a similar way:

$$H_{\mathrm{HP}}=-2JNZS^2(1+\zeta\nu)+2JZS\sum_k[\{1+\zeta\nu(1-\gamma_k')\}(a_k^+a_k+b_k^+b_k)$$
$$+\gamma_k(a_kb_k+a_k^+b_k^+)]-2JZN^{-1}\sum_{k1,k2,k3}[\gamma_{k1-k2}a_{k1}^+a_{k2}b_{k3}^+b_{-k1+k2+k3}$$
$$+\frac{1}{4}\{\gamma_{-k1+k2-k3}(a_{k1}^+a_{k2}a_{k3}b_{-k1+k2+k3}+a_{k1}^+a_{-k2}^+a_{k3}b_{k1-k2-k3}^+)$$
$$+\gamma_{k1}(a_{k1}b_{k2}^+b_{k3}b_{k1+k2-k3}+a_{k1}^+b_{k2}^+b_{k3}^+b_{-k1+k2+k3})\}]. \tag{7}$$

The Hamiltonians (4) and (7) take the same form in the harmonic approximation as follows:

$$H=-2JNZS^2(1+\zeta\nu)+2JZS\sum_k[\{1+\zeta\nu(1-\gamma_k')\}(a_k^+a_k+b_k^+b_k)$$
$$+\gamma_k(a_kb_k+a_k^+b_k^+)]. \tag{8}$$

The Bogoliubov transformation is introduced to make the Hamiltonian (8) diagonal:

$$\alpha_k=u_ka_k-v_kb_k^+, \text{ and } \beta_k=u_kb_k-v_ka_k^+, \tag{9}$$

then the energy of a spin wave is given as follows:

$$\lambda_k=2JSZ[\{1+\zeta\nu(1-\gamma_k')\}^2-\gamma_k^2]^{1/2}, \tag{10}$$

where

$$u_k = \pm\left[2JSZ\{1+\zeta\nu(1-\gamma_k')\}/2\lambda_k+\frac{1}{2}\right]^{1/2},$$

and

$$v_k = \mp\left[2JSZ\{1+\zeta v(1-\gamma_k')\}/2\lambda_k-\frac{1}{2}\right]^{1/2}. \tag{11}$$

Next, we shall treat the chain-like antiferromagnet with the antiferromagnetic inter-chain interaction and the Hamiltonian is represented by

$$H'=2J\sum_{j,l>}\boldsymbol{S}_j\cdot\boldsymbol{S}_l+2J'\sum_{m,n>}\boldsymbol{S}_m\cdot\boldsymbol{S}_n, \tag{12}$$

where m and n represent pairs of sites in different sublattices in this case. The Hamiltonian (12) can be written in the forms which correspond to equations (4) and (7) as follows:

$$\begin{aligned}H'_{\mathrm{DM}}=&-2JNZS^2(1+\zeta\nu)+2JZS\sum_k\{a_k^\dagger a_k+b_k^\dagger b_k+\gamma_k(a_kb_k+a_k^\dagger b_k^\dagger)\}\\&+2J'Z'S\sum_k\{a_k^\dagger a_k+b_k^\dagger b_k+\gamma_k'(a_kb_k+a_k^\dagger b_k^\dagger)\}\\&-2JZN^{-1}\sum_{k1,k2,k3}[\gamma_{k1-k2}a_{k1}^\dagger a_{k2}b_{k3}^\dagger b_{-k1+k2-k3}\\&+\frac{1}{2}(\gamma_{-k1+k2+k3}a_{k1}^\dagger a_{k2}a_{k3}b_{-k1+k2+k3}+\gamma_{k1}a_{k1}b_{k2}^\dagger b_{k3}b_{k1+k2-k3})],\end{aligned} \tag{13}$$

and

$$\begin{aligned}H'_{\mathrm{HP}}=&-2JNZS^2(1+\zeta\nu)+2JZS\sum_k\{a_k^\dagger a_k+b_k^\dagger b_k+\gamma_k(a_kb_k+a_k^\dagger b_k^\dagger)\}\\&+2J'Z'S\sum_k\{a_k^\dagger a_k+b_k^\dagger b_k+\gamma_k(a_kb_k+a_k^\dagger b_k^\dagger)\}\\&-2JZN^{-1}\sum_{k1,k2,k3}[\gamma_{k1-k2}a_{k1}^\dagger a_{k2}b_{k3}^\dagger b_{-k1+k2+k3}\\&+\frac{1}{4}\{\gamma_{-k1+k2+k3}(a_{k1}^\dagger a_{k2}a_{k3}b_{-k1+k2+k3}+a_{k1}^\dagger a_{-k2}^\dagger a_{k3}b_{k1-k2-k3}^\dagger)\\&+\gamma_{k1}(a_{k1}b_{k2}^\dagger b_{k3}b_{k1+k2-k3}+a_{k1}^\dagger b_{k2}^\dagger b_{k3}^\dagger b_{-k1+k2+k3})\}].\end{aligned} \tag{14}$$

The excitation energy of a spin wave is obtained in the harmonic approximation:

$$\lambda_k'=2JZS\{(1+\zeta\nu)^2-(\gamma_k+\zeta\nu\gamma_k')^2\}^{1/2}. \tag{15}$$

The spin reduction ΔS is given (FUKUCHI and OKABE 1977):

$$\Delta S_{\mathrm{M}}=v-\frac{\sum_{u=1}^{2S}D_u(1+u)(1+v)^{-(1+u)}v^{1+u}}{1-\sum_{u=1}^{2S}D_u(1+v)^{-(1+u)}v^{1+u}}, \tag{16}$$

or

$$\Delta S_{\mathrm{P}}=v-\frac{(2S+1)v^{2S+1}}{(1+v)^{2S+1}-v^{2S+1}}, \tag{17}$$

where

$$D_u = F_u - F_{u-1},\quad F_u = 1\cdot(1-1/2S)\cdots\{1-(u-1)/2S\},$$
$$\text{and}\quad v = N^{-1}\sum_k v_k^2, \tag{18}$$

where v_k is the coefficient which appears in the Bogoliubov transformation.

The numerical values of ΔS in the case of ferromagnetic inter-chain interaction are given in Table 1 (a). Figure 1 shows the reduction for $S=1$ and $S=5/2$, where the solid lines represent the results obtained from equation (16), the broken lines from equation (17) and the results of the usual free spin wave theory are also shown with the chain line. Table 1 (b) shows the reduction in the case of antiferromagnetic interchain interaction. The difference of ΔS between both cases is considerably small as is clearly seen in Table 1.

Table 1. Zero-point spin reduction obtained in the harmonic approximation; (a) the inter-chain interaction J' is ferromagnetic and (b) J' antiferromagnetic. The values of ΔS_M and ΔS_P are given by equations (16) and (17) respectively.

(a) J' : ferromagnetic

	ΔS_M				
	S				
J'/J	1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0743	0.0801	0.0823	0.0834	0.0842
1×10^{-1}	0.1379	0.1582	0.1670	0.1720	0.1752
3.16×10^{-2}	0.2000	0.2440	0.2655	0.2785	0.2872
1×10^{-2}	0.2499	0.3198	0.3573	0.3812	0.3981
3.16×10^{-3}	0.2874	0.3812	0.4350	0.4709	0.4969
1×10^{-4}	0.3157	0.4300	0.4988	0.5464	0.5817
3.16×10^{-4}	0.3375	0.4692	0.5513	0.6096	0.6539
1×10^{-4}	0.3548	0.5010	0.5949	0.6629	0.7154

	ΔS_P				
	S				
J'/J	1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0743	0.0857	0.0871	0.0873	0.0873
1×10^{-1}	0.1379	0.1780	0.1877	0.1898	0.1902
3.16×10^{-2}	0.2000	0.2858	0.3177	0.3285	0.3319
1×10^{-2}	0.2499	0.3843	0.4496	0.4788	0.4912
3.16×10^{-3}	0.2874	0.4652	0.5671	0.6219	0.6499
1×10^{-3}	0.3157	0.5298	0.6667	0.7498	0.7981
3.16×10^{-4}	0.3375	0.5815	0.7497	0.8610	0.9320
1×10^{-4}	0.3548	0.6234	0.8191	0.9569	1.0510

(b) J': antiferromagnetic

J'/J	ΔS_M				
	S				
	1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0877	0.0957	0.0989	0.1006	0.1016
1×10^{-1}	0.1411	0.1624	0.1718	0.1771	0.1805
3.16×10^{-2}	0.2007	0.2450	0.2667	0.2998	0.2887
1×10^{-2}	0.2500	0.3200	0.3576	0.3816	0.3984
3.16×10^{-3}	0.2874	0.3812	0.4350	0.4709	0.4970
1×10^{-3}	0.3157	0.4301	0.4988	0.5464	0.5818
3.16×10^{-4}	0.3375	0.4692	0.5513	0.6096	0.6539
1×10^{-4}	0.3548	0.5010	0.5949	0.6629	0.7154

J'/J	ΔS_P				
	S				
	1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0877	0.1036	0.1060	0.1063	0.1063
1×10^{-1}	0.1411	0.1832	0.1937	0.1960	0.1965
3.16×10^{-2}	0.2007	0.2871	0.3149	0.3304	0.3339
1×10^{-2}	0.2500	0.3846	0.4500	0.4793	0.4918
3.16×10^{-3}	0.2874	0.4653	0.5673	0.6220	0.6501
1×10^{-3}	0.3157	0.5299	0.6667	0.7498	0.7982
3.16×10^{-4}	0.3375	0.5815	0.7497	0.8610	0.9320
1×10^{-4}	0.3548	0.6234	0.8191	0.9569	1.0510

§ 3. Dynamical Interaction

In order to treat the contribution due to the dynamical interaction, we shall consider in this section the biquadratic terms of the boson operators in the mean field approximation. The equations of motion for a_k and b_k^+ can be obtained from Hamiltonian (4):

$$i(\partial/\partial t)a_k = \Gamma_k a_k + \Lambda_{1k} b_k^+,$$

and

$$i(\partial/\partial t)b_k^+ = -\Gamma_k b_k^+ - \Lambda_{2k} a_k, \tag{19}$$

where

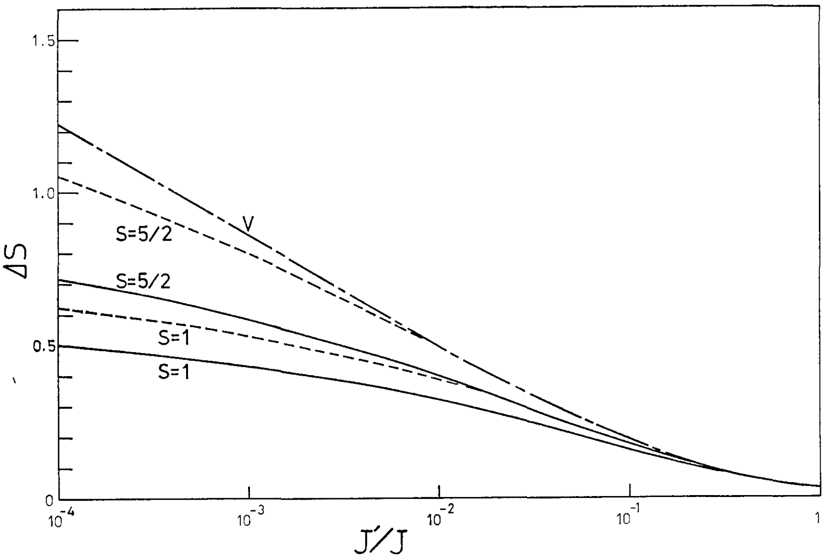

Fig. 1. Zero-point spin reduction with ferromagnetic inter-chain interaction for $S=1$ and $S=5/2$ in the harmonic approximation. Solid lines and broken lines correspond to ΔS_{M} and ΔS_{P} respectively, and a chain line to v which does not depend on the magnitude of S.

$$\Gamma_k=2JZS[1+\zeta\nu(1-\gamma_k')-(SN)^{-1}\sum_{\mu}\{(a_\mu^+ a_\mu)+\gamma_\mu(a_\mu b_\mu)\}],$$

$$\Delta_{1k}=2JZS[1-(SN)^{-1}\sum_{\mu}\gamma_\mu(a_\mu b_\mu)]\gamma_k,$$

and

$$\Delta_{2k}=2JZS[1-(SN)^{-1}\sum_{\mu}\{2(a_\mu^+ a_\mu)+\gamma_\mu(a_\mu b_\mu)\}]\gamma_k. \tag{20}$$

Here, interaction terms are linearized by replacing pairs of boson operators by their expectation values in the ground state and the following relations between these expectation values are used in equation (20);

$$(a_k^+ a_k)=(b_k^+ b_k), \quad (a_k b_k)=(a_k^+ b_k^+), \quad \text{and} \quad \gamma_{k+k'}=\gamma_k\gamma_{k'}\,.$$

Further, Δ_{1k} and Δ_{2k} are replaced by their arithmetical mean value Δ_k to get the effective Hamiltonian:

$$H_{eff}=-2JNZS^2(1+\zeta\nu)+\sum_k \Gamma_k(a_k^+ a_k+b_k^+ b_k)$$
$$+\sum_k \Delta_k(a_k b_k+a_k^+ b_k^+),$$

and

$$\Delta_k=2JZS[1-(SN)^{-1}\sum_{\mu}\{(a_\mu^+ a_\mu)+\gamma_\mu(a_\mu b_\mu)\}]\gamma_k. \tag{21}$$

The equations of motion obtained from the Hamiltonian (7) give the same Hamiltonian (21) in this approximation.

The Bogoliubov transformation is introduced to get the renormalized spin wave energy:

$$\lambda_k = 2JZS[\{1+\zeta\nu(1-\gamma_k') - \Delta/S\}^2 - (1-\Delta/S)^2\gamma_k^2]^{1/2}, \tag{22}$$

where

$$\Delta = N^{-1}\sum_{\mu}\{(a_\mu^+ a_\mu) + \gamma_\mu(a_\mu b_\mu)\}. \tag{23}$$

Here, Δ should be determined self-consistently. The numerical calculation shows the convergence is obtained by a few times of iterations. The results are shown in Table 2 (a).

The Hamiltonians (13) and (14) with antiferromagnetic inter-chain coupling give the same effective Hamiltonian in the same way mentioned above:

$$H'_{eff} = -2JNZS^2(1+\zeta\nu) + \sum_k \Gamma_k'(a_k^+ a_k + b_k^+ b_k) + \sum_k \Lambda_k'(a_k b_k + a_k^+ b_k^+), \tag{24}$$

Table 2. Values of Δ which are obtained self-consistently by several times of interations.

(a) Δ (J': ferromagnetic)

J'/J	S = 1/2	1	3/2	2	5/2
3.16×10^{-1}	−0.1328	−0.1291	−0.1277	−0.1270	−0.1266
1×10^{-1}	−0.1621	−0.1598	−0.1589	−0.1584	−0.1581
3.16×10^{-2}	−0.1748	−0.1738	−0.1735	−0.1733	−0.1731
1×10^{-2}	−0.1794	−0.1791	−0.1789	−0.1789	−0.1788
3.16×10^{-3}	−0.1810	−0.1808	−0.1808	−0.1808	−0.1808
1×10^{-3}	−0.1815	−0.1814	−0.1814	−0.1814	−0.1814
3.16×10^{-4}	−0.1816	−0.1816	−0.1816	−0.1816	−0.1816
1×10^{-4}	−0.1817	−0.1817	−0.1817	−0.1817	−0.1817

(b) Δ (J': antiferromagnetic)

J'/J	S = 1/2	1	3/2	2	5/2
3.16×10^{-1}	−0.1252	−0.1204	−0.1188	−0.1179	−0.1174
1×10^{-1}	−0.1608	−0.1582	−0.1572	−0.1567	−0.1563
3.16×10^{-2}	−0.1746	−0.1736	−0.1732	−0.1730	−0.1729
1×10^{-2}	−0.1794	−0.1791	−0.1789	−0.1788	−0.1788
3.16×10^{-3}	−0.1810	−0.1808	−0.1808	−0.1808	−0.1808
1×10^{-3}	−0.1815	−0.1814	−0.1814	−0.1814	−0.1814
3.16×10^{-4}	−0.1816	−0.1816	−0.1816	−0.1816	−0.1816
1×10^{-4}	−0.1817	−0.1817	−0.1817	−0.1817	−0.1817

Table 3. Spin reduction v given by equation (18). (a) J' is ferromagnetic and (b) J' antiferromagnetic. The 2nd column represents the values of v obtained in the harmonic approximation, and the 3rd∼7th columns correspond to those in the renormalized treatment.

(a) J' : ferromagnetic

J'/J	Harmonic	S				
		1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0873	0.1045	0.0959	0.0930	0.0916	0.0907
1×10^{-1}	0.1903	0.2222	0.2069	0.2015	0.1988	0.1971
3.16×10^{-2}	0.3334	0.3751	0.3555	0.3485	0.3448	0.3426
1×10^{-2}	0.4994	0.5457	0.5242	0.5164	0.5123	0.5098
3.16×10^{-3}	0.6758	0.7241	0.7018	0.6936	0.6893	0.6867
1×10^{-3}	0.8565	0.9045	0.8828	0.8745	0.8702	0.8676
3.16×10^{-4}	1.0388	1.0880	1.0653	1.0569	1.0526	1.0499
1×10^{-4}	1.2216	1.2709	1.2482	1.2398	1.2354	1.2328

(b) J' : antiferromagnetic

J'/J	Harmonic	S				
		1/2	1	3/2	2	5/2
3.16×10^{-1}	0.1063	0.1190	0.1125	0.1104	0.1093	0.1087
1×10^{-1}	0.1966	0.2267	0.2121	0.2071	0.2045	0.2029
3.16×10^{-2}	0.3354	0.3765	0.3571	0.3502	0.3466	0.3444
1×10^{-2}	0.5000	0.5462	0.5247	0.5169	0.5128	0.5103
3.16×10^{-3}	0.6760	0.7242	0.7019	0.6937	0.6895	0.6869
1×10^{-3}	0.8566	0.9055	0.8829	0.8746	0.8703	0.8676
3.16×10^{-4}	1.0388	1.0880	1.0653	1.0570	1.0526	1.0500
1×10^{-4}	1.2216	1.2709	1.2482	1.2398	1.2354	1.2328

where

$$\Gamma_k' = 2JZS(1+\zeta\nu-\Delta'/S), \quad \Lambda_k' = 2JZS(\gamma_k+\zeta\nu\gamma_k'-\Delta'\gamma_k/S),$$

and

$$\Delta' = N^{-1}\sum_{\mu}\{(a_\mu^+a_\mu)+\gamma_\mu(a_\mu b_\mu)\}. \tag{25}$$

Then the spin wave energy is given by

$$\lambda_k' = (\Gamma_k'^2-\Lambda_k'^2)^{1/2}. \tag{26}$$

Here also Δ' should be calculated self-consistently and the results are given in Table 2(b). It is seen in Table 2 that Δ and Δ' approach to a finite value which seems to show no dependence upon S when ζ tends to zero. Further, Table 2 shows that the difference between the energy spectra of spin waves, (22) and (26), is small. It is concluded that the spin wave spectrum is not so seriously affected by the inter-chain interaction even if it is ferromagnetic or antiferromagnetic.

In Table 3, there are shown both of the values of v in the usual free spin wave theory and the values in the approximations when the biquadratic terms are treated self-consistently; (a) J' is ferromagnetic and (b) J' antiferromagnetic. The contribution due to dynamical interaction is not so large within our approximations at least, when ζ decreases, namely, the chain-like property predominates. The large spin reduction in the chain-like antiferromagnets can, therefore, be mainly attributed to kinematical interaction. Table 4 shows the values of zero-point spin reduction when the dynamical interaction is considered for the cases of ferromagnetic and antiferromagnetic inter-chain exchange coupling.

Table 4. Zero-point spin reduction obtained in the renormalized spin wave treatment. (a) J' is ferromagnetic and (b) J' antiferromagnetic. The values of ΔS_M and ΔS_P are given by equations (16) and (17) respectively.

(a) J' : ferromagnetic

J'/J	ΔS_M				
	S				
	1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0864	0.0872	0.0873	0.0873	0.0873
1×10^{-1}	0.1538	0.1693	0.1754	0.1788	0.1809
3.16×10^{-2}	0.2143	0.2553	0.2747	0.2862	0.2939
1×10^{-2}	0.2609	0.3294	0.3655	0.3884	0.4404
3.16×10^{-3}	0.2958	0.3890	0.4418	0.4770	0.5024
1×10^{-3}	0.3221	0.4362	0.5045	0.5515	0.5865
3.16×10^{-4}	0.3426	0.4742	0.5560	0.6140	0.6579
1×10^{-4}	0.3588	0.5051	0.5988	0.6666	0.7189

J'/J	ΔS_P				
	S				
	1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0864	0.0939	0.0928	0.0916	0.0907
1×10^{-1}	0.1538	0.1917	0.1983	0.1982	0.1970
3.16×10^{-2}	0.2143	0.3004	0.3306	0.3393	0.3409
1×10^{-2}	0.2609	0.3970	0.4619	0.4899	0.5009
3.16×10^{-3}	0.2958	0.4755	0.5778	0.6321	0.6593
1×10^{-3}	0.3221	0.5380	0.6756	0.7587	0.8067
3.16×10^{-4}	0.3427	0.5881	0.7572	0.8688	0.9396
1×10^{-4}	0.3588	0.6288	0.8254	0.9636	1.0579

(b) J' : antiferromagnetic

J'/J	ΔS_M, S = 1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0961	0.1006	0.1024	0.1033	0.1038
1×10^{-1}	0.1560	0.1727	0.1796	0.1834	0.1858
3.16×10^{-2}	0.2148	0.2561	0.2757	0.2874	0.2952
1×10^{-2}	0.2610	0.3296	0.3658	0.3887	0.4047
3.16×10^{-3}	0.2958	0.3890	0.4419	0.4771	0.5025
1×10^{-3}	0.3221	0.4363	0.5045	0.5516	0.5865
3.16×10^{-4}	0.3426	0.4742	0.5560	0.6140	0.6579
1×10^{-4}	0.3588	0.5051	0.5988	0.6666	0.7189

J'/J	ΔS_P, S = 1/2	1	3/2	2	5/2
3.16×10^{-1}	0.0961	0.1094	0.1100	0.1093	0.1087
1×10^{-1}	0.1560	0.1954	0.2036	0.2038	0.2028
3.16×10^{-2}	0.2148	0.3014	0.3320	0.3409	0.3427
1×10^{-2}	0.2610	0.3972	0.4622	0.4903	0.5014
3.16×10^{-3}	0.2958	0.4756	0.5579	0.6322	0.6594
1×10^{-3}	0.3221	0.5381	0.6756	0.7588	0.8067
3.16×10^{-4}	0.3426	0.5881	0.7572	0.8688	0.9397
1×10^{-4}	0.3588	0.6288	0.8254	0.9636	1.0579

§ 4. Discussion

Now we shall consider the relation between our metric operator method and the projection operator method. The j-th lattice site is considered and we shall drop the site-index j hereafter. In the metric operator method, an operator A in the spin space is represented as follows (MILLS and KENAN 1966):

$$A=\sum_{u,v}|u>\frac{1}{F_u}\langle u|A|v\rangle\frac{1}{F_v}<v|. \tag{27}$$

The corresponding operator in the boson space can be written as

$$\hat{A}_{\mathrm{DM}}=\sum_{u,v}|u)\frac{1}{F_u}(u|\eta\hat{A}_{\mathrm{DM}}|v)\frac{1}{F_v}(v|\eta. \tag{28}$$

Thus, these operators satisfy the relation;

$$\langle u|A|v\rangle=(u|\eta\hat{A}_{\mathrm{DM}}|v). \tag{29}$$

Because the metric operator appears as the form $\eta\hat{A}_{\mathrm{DM}}$ in the right hand side of equation (29), the summations over u and v are restricted naturally to the physical states only. On the other hand, if we take the orthonormal basis in the spin space, $|u'\rangle=F_u^{-1/2}|u\rangle$, the operator A is expressed as follows:

$$A=\sum_{u',v'}|u'\rangle\langle u'|A|v'\rangle\langle v'|,$$

and

$$\hat{A}_{\mathrm{HP}}=\sum_{u',v'}|u')(u'|P\hat{A}_{\mathrm{HP}}|v')(v'|P. \tag{30}$$

Then, the relation $\langle u'|A|v'\rangle=(u'|P\hat{A}_{\mathrm{HP}}|v')$ holds. As this relation is defined in terms of the orthonormal basis, the metric operator does not appear apparently. It is necessary, however, to introduce the projection operator P to exclude contributions arising from nonphysical states. It is possible to confirm that $\hat{A}_{\mathrm{DM}}$ and $\hat{A}_{\mathrm{HP}}$ are the DM- and HP-operator respectively, corresponding to the operator A in the spin space.

If the exact ground state $|\tilde{O})_{\mathrm{DM}}$ in the boson space is obtained by DM-transformation, it can be represented as

$$|\tilde{O})_{\mathrm{DM}}=\sum_{n=0}^{2S}d_n|n)_{\mathrm{DM}}. \tag{31}$$

The corresponding state $|\tilde{O}\rangle$ in the spin space is expressed by

$$|\tilde{O}\rangle=\sum_{n=0}^{2S}d_n|n\rangle. \tag{32}$$

As the matrix elements are related by (29), the spin reduction ΔS is given by

$$\Delta S_{\mathrm{DM}}=\sum_{n=0}^{2S}d_n^2\cdot F_n\cdot n/\sum_{n=0}^{2S}d_n^2\cdot F_n. \tag{33}$$

On the other hand, if the exact ground state $|\tilde{O})_{\mathrm{HP}}$ is obtained by HP-transformation, it should be written as

$$|\tilde{O})_{\mathrm{HP}}=\sum_{n'=0}^{2S}h_{n'}|n')_{\mathrm{HP}}. \tag{34}$$

Since $|n')_{\mathrm{HP}}$ corresponds to the normalized spin state, ΔS becomes

$$\Delta S_{\mathrm{HP}}=\sum_{n'=0}^{2S}h_{n'}^2\cdot n'/\sum_{n'=0}^{2S}h_{n'}^2. \tag{35}$$

It is seen from these results, (33) and (35), that there is an apparent effect of kinematical interaction even in the physial states in DM. It seems that this causes the spin reduction ΔS_{M} smaller than that of ΔS_{P} in the numerical calculation. The difference between $|\tilde{O})_{\mathrm{DM}}$ and $|\tilde{O})_{\mathrm{HP}}$ does not come out in our present approximation, and therefore the further investigations (treatment of source terms, and of non-Hermitian nature of H_{DM}, etc.) are necessary to clear up the difference of the two. These problems have to be solved in future.

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