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Author	福地, 充(Fukuchi, Mitsuru) 原田, 政次(Harada, Masaji)
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# Energy of the Spin Wave in an Antiferromagnet

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Mitsuru FUKUCHI\*

Masaji HARADA\*\*

## Abstract

The isotropic Heisenberg model for an antiferromagnetic crystal is investigated on the basis of spin wave theory. Theory for the free spin waves are developed by the Bogolyubov transformation and by the approach with the use of the equation of motion. The effects of mutual interaction between spin waves in the equation of motion are investigated approximately with the self-consistent treatment for the interaction at low temperature. The resulting temperature dependent spin wave energies are examined together with the temperature variation of the reduction of sublattice magnetization. Relation to the approach by the Green function method are considered briefly.

## I. Introduction

The spin wave, namely the elementary excitation near the magnetic ground state is one of the concepts of great value and of considerable importance in the theory of magnetism. We can obtain the information about the condition for stability of ground states as well as the knowledge about the excitation spectra. For the ferromagnetic Heisenberg model, we have the famous Dyson's theory on spin waves and their interactions.<sup>1)</sup> A spin wave quantum is a well defined quasi-particle near the ground state, which can be interpreted qualitatively by so called free spin wave Hamiltonian. This Hamiltonian is expressed within the second order terms in spin wave annihilation and creation operators. The higher order Hamiltonian consists of interaction terms between spin waves, one of the direct physical consequences of which seems to be the temperature variation of elementary excitation energies.

In our present work we consider an antiferromagnet in Heisenberg model treating the effects of interaction self-consistently using the linearization approach of the equation of motion, although we have studied a ferromagnet in a localized model in greater detail by means of Green function approach in our previous work.<sup>2)</sup> As for the starting antiferromagnetic spin Hamiltonian we take,

$$\mathcal{H} = 2|J| \sum_{\langle i, m \rangle} S_i \cdot S_m - g\mu_B H (\sum_i S_i^z + \sum_m S_m^z), \quad (1-1)$$

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\*福地 充 Associate Professor, Faculty of Engineering, Keio University.

\*\*原田 政次 Graduate Student, Faculty of Engineering, Keio University.

where  $S_l$  and  $S_m$  refer to spin operators at lattice site  $l$  and  $m$  respectively and  $H$  represents the externally applied magnetic field, which is assumed to be along  $+z$ -direction. The subscript  $\langle l, m \rangle$  under the summation symbol means that  $l$  and  $m$  are restricted to nearest neighbor pairs and the summation is carried out over the set of pairs. We use the symbol  $\mu_B$  for the Bohr magneton, and  $g$  for the Landé  $g$ -factor of a magnetic atom in a crystal. We take the usual two sublattice model for an antiferromagnet, that is, a lattice site  $l$  belongs to sublattice  $A$  and a lattice site  $m$  belongs to sublattice  $B$  respectively. We assume that the nearest neighbors of the  $A$  (or  $B$ ) site are the members of the  $B$  (or  $A$ ) sublattice and the nearest neighbor antiferromagnetic coupling of strength  $J$ , which is assumed to be negative. We consider that our crystal contains  $2N$  magnetic atoms in all. In the Hamiltonian (1-1) we neglect any anisotropic field which is of importance in a real antiferromagnetic crystal. In other words we consider the limiting case in which the anisotropic field becomes infinitely small. We have main interests with the behaviour of an antiferromagnet with no anisotropy, and further we assume the applied field  $H$  to be very weak and do not treat the problem of instability for a strong field or for the direction of field in the present work.

The Néel state, which we denote as the ordered antiparallel spin state and which is not an exact eigen state of our Hamiltonian (1-1) is assumed to be an approximate ground state. Thus each spin in the  $A$ -sublattice is in a state of  $S_l^z = +S$ , and each spin in the  $B$ -sublattice is in a state of  $S_m^z = -S$ , respectively. Starting from the Néel state above mentioned, we express the spin operators in terms of Boson operators  $a_l, a_l^+, b_m^+$  and  $b_m$  as follows,

$$\begin{aligned}
 S_l^+ &= \sqrt{2S} \left( 1 - \frac{a_l^+ a_l}{2S} \right) a_l \\
 S_l^- &= \sqrt{2S} a_l^+ \\
 S_l^z &= S - a_l^+ a_l \\
 S_m^+ &= \sqrt{2S} b_m^+ \left( 1 - \frac{b_m^+ b_m}{2S} \right) \\
 S_m^- &= \sqrt{2S} b_m \\
 S_m^z &= -S + b_m^+ b_m,
 \end{aligned} \tag{1-2}$$

where  $a_l$  and  $a_l^+$  refer to the spin deviation of lattice site  $l$  in the  $A$ -sublattice and  $b_m^+$  and  $b_m$  refer to that of lattice site  $m$  in the  $B$ -sublattice respectively. Operators  $a_l, a_l^+, b_m^+$  and  $b_m$  obey the well-known commutation relations.

$$\begin{aligned}
 [a_l, a_l^+] &= \delta_{l, l'} \\
 [b_m, b_m'^+] &= \delta_{m, m'} \\
 \text{Other commutators} &\text{ are zero.}
 \end{aligned} \tag{1-3}$$

We obtain the Hamiltonian of idealized spin-type<sup>1)</sup> using the transformation (1-2) as follows,

$$(32)$$

$$\begin{aligned}
\mathcal{H} = & -2z|J|NS^2 \\
& + g\mu_B H \left\{ \sum_l a_l^+ a_l - \sum_m b_m^+ b_m \right\} + 2|J|S \sum_{\langle l,m \rangle} \{ a_l^+ a_l + b_m^+ b_m + a_l b_m + a_l^+ b_m^+ \} \\
& - |J| \sum_{\langle l,m \rangle} \{ a_l^+ a_l a_l b_m + a_l^+ b_m^+ b_m^+ b_m + 2a_l^+ a_l b_m^+ b_m \}. \tag{1-4}
\end{aligned}$$

This Hamiltonian is expressed in terms of localized spin deviation operators  $a_l$ ,  $a_l^+$ ,  $b_m^+$  and  $b_m$ . In order to change the representation into the wave number space we introduce the spin wave operators with wave vector  $\kappa$ , namely  $a_\kappa$ ,  $a_\kappa^+$ ,  $b_\kappa$  and  $b_\kappa^+$  defined as follows,

$$\begin{aligned}
a_l &= \frac{1}{\sqrt{N}} \sum_\kappa a_\kappa e^{il \cdot \kappa} & a_l^+ &= \frac{1}{\sqrt{N}} \sum_\kappa a_\kappa^+ e^{-il \cdot \kappa} \\
b_m &= \frac{1}{\sqrt{N}} \sum_\kappa b_\kappa e^{-im \cdot \kappa} & b_m^+ &= \frac{1}{\sqrt{N}} \sum_\kappa b_\kappa^+ e^{im \cdot \kappa}. \tag{1-5}
\end{aligned}$$

The different choice for the sign of the exponent corresponds to the different choice of the annihilation and creation operators for  $S^-$  and  $S^+$  in the equations (1-2). Then we obtain the required spin wave Hamiltonian.

$$\begin{aligned}
\mathcal{H} = & -2z|J|NS^2 + g\mu_B H \sum_\kappa (a_\kappa^+ a_\kappa - b_\kappa^+ b_\kappa) \\
& + 2|J|S z \sum_\kappa (a_\kappa^+ a_\kappa + b_\kappa^+ b_\kappa + \mathcal{F}_\kappa a_\kappa b_\kappa + \mathcal{F}_\kappa^* a_\kappa^+ b_\kappa^+) \\
& - \frac{1}{N} z |J| \sum_{\kappa_1, \kappa_2, \kappa_3, \kappa_4} (\mathcal{F}_{\kappa_1} a_{\kappa_1}^+ a_{\kappa_2} a_{\kappa_3} b_{\kappa_4} + \mathcal{F}_{\kappa_1}^* a_{\kappa_1}^+ b_{\kappa_2}^+ b_{\kappa_3}^+ b_{\kappa_4}) \\
& + 2\mathcal{F}_{\kappa_3 - \kappa_4} a_{\kappa_1}^+ a_{\kappa_2} b_{\kappa_3}^+ b_{\kappa_4}) \delta(\kappa_1 - \kappa_2 - \kappa_3 + \kappa_4) \tag{1-6}
\end{aligned}$$

and

$$\mathcal{F}_\kappa = \frac{1}{z} \sum_{\delta} e^{i\delta \cdot \kappa}, \tag{1-7}$$

where the summation over the vector  $\delta$  is carried out only for the  $z$ -vectors that connect an atom with its  $z$ -neighbors.

Our transformed Hamiltonian (1-4) or (1-6) equivalently contains unphysical states as well as physical ones. This makes the problem essentially difficult when we treat it at arbitrary temperature. We consider, however, the behaviour in low temperature region only, where the contribution of unphysical states to various physical quantities at temperature  $T^\circ\text{K}$  is vanishingly small with the factor proportional to  $\exp\left(-\frac{\Delta}{kT}\right)$ , owing to the fact that we may have a finite energy gap  $\Delta$  between the lowest physical and the lowest unphysical eigenstates of our Hamiltonian (1-6).

## II. Treatment of the Hamiltonian for the free spin waves

In this paragraph we treat the second order part of the Hamiltonian (1-6), in which modes of different wave vectors do not interact with each other. Thus

we may consider the following part referring to wave vector  $\kappa$  in the Hamiltonian (1-6),

$$\mathscr{H}^{II}(\kappa) = \varepsilon_1(\kappa)a_\kappa^+a_\kappa + \varepsilon_2(\kappa)b_\kappa^+b_\kappa + \gamma(\kappa)(a_\kappa b_\kappa + a_\kappa^+b_\kappa^+) \quad (2-1)$$

and omit the wave number vector  $\kappa$  for a while. We notice,

$$\varepsilon_1(\kappa) = 2z|J|S + g\mu_B H, \quad \varepsilon_2(\kappa) = 2z|J|S - g\mu_B H$$

and 
$$\gamma(\kappa) = 2z|J|\mathcal{F}(\kappa). \quad (2-2)$$

Usually the terms of pair-creation and annihilation operators are eliminated by the Bogolyubov transformation<sup>4)</sup>, in which operators  $a$ 's and  $b$ 's are expressed in terms of new Boson operators  $\alpha$ 's and  $\beta$ 's,

$$\begin{aligned} a &= e\alpha + s\beta^+ & a^+ &= e\alpha^+ + s\beta \\ b &= s\alpha^+ + e\beta & b^+ &= s\alpha + e\beta^+. \end{aligned} \quad (2-3)$$

In order that new operators  $\alpha$ 's and  $\beta$ 's should represent Boson operators, that is, they should satisfy the same type of commutation relations as the equations (1-3), the coefficients  $e$  and  $s$  which are assumed to be real numbers here, must satisfy the following relation,

$$e^2 - s^2 = 1. \quad (2-4)$$

The new Hamiltonian expressed in terms of  $\alpha$  and  $\beta$  should have the vanishing coefficients for the terms  $\alpha\beta$  and  $\alpha^+\beta^+$ , thus we obtain the following condition,

$$(\varepsilon_1 + \varepsilon_2)es + \gamma(e^2 + s^2) = 0. \quad (2-5)$$

Equations (2-4) and (2-5) determine the coefficients of Bogolyubov transformation  $e$  and  $s$  together with the requirement that  $\alpha$  should tend to  $a$  and  $\beta$  to  $b$  for small  $\gamma$ ,

$$e^2 = \frac{1}{2} \left\{ \frac{1}{\sqrt{1 - \left(\frac{\gamma}{\varepsilon}\right)^2}} + 1 \right\}, \quad 2es = - \frac{\frac{\gamma}{\varepsilon}}{\sqrt{1 - \left(\frac{\gamma}{\varepsilon}\right)^2}},$$

and 
$$s^2 = \frac{1}{2} \left\{ \frac{1}{\sqrt{1 - \left(\frac{\gamma}{\varepsilon}\right)^2}} - 1 \right\} \quad (2-6)$$

where we have introduced the quantity  $\varepsilon$  that is defined by

$$\varepsilon = \frac{1}{2} (\varepsilon_1 + \varepsilon_2). \quad (2-7)$$

Thus we obtain the following Hamiltonian in terms of  $\alpha$ 's and  $\beta$ 's,

$$\mathscr{H}^{II}(\kappa) = E_0 + \tilde{\varepsilon}_1 \alpha^+ \alpha + \tilde{\varepsilon}_2 \beta^+ \beta \quad (2-8)$$

where

$$E_0 = s^2 (\varepsilon_1 + \varepsilon_2) + 2es\gamma = \varepsilon \left\{ \sqrt{1 - \left(\frac{\gamma}{\varepsilon}\right)^2} - 1 \right\} \quad (2-9)$$

$$\tilde{\varepsilon}_1 = \varepsilon_1 e^2 + \varepsilon_2 s^2 + 2es\gamma = \varepsilon \sqrt{1 - \left(\frac{\gamma}{\varepsilon}\right)^2} + \frac{1}{2} (\varepsilon_1 - \varepsilon_2) \quad (2-10)$$

and

$$\tilde{\varepsilon}_2 = \varepsilon_1 s^2 + \varepsilon_2 e^2 + 2es\gamma = \varepsilon \sqrt{1 - \left(\frac{\gamma}{\varepsilon}\right)^2} - \frac{1}{2} (\varepsilon_1 - \varepsilon_2). \quad (2-11)$$

Now we will treat the same problem along the view-point of the equation of motion approach. In order to examine the time-rate of change of  $a$  and  $b^+$  quantum mechanically, we must take commutators  $a$  and  $b^+$  with  $\mathcal{H}^{II}$ , to get

$$\begin{aligned} [a, \mathcal{H}^{II}] &= \varepsilon_1 a + \gamma b^+ \\ [b^+, \mathcal{H}^{II}] &= -\gamma a - \varepsilon_2 b^+. \end{aligned} \quad (2-12)$$

Equations (2-12) show that coordinate  $a$  couples with coordinate  $b^+$  and that the normal coordinate should be a linear combination of  $a$  and  $b^+$ . Thus we seek the normal coordinate in the form,  $\alpha = ea - sb^+$  with the requirement that  $[\alpha, \mathcal{H}^{II}]$  equals to  $+\tilde{\varepsilon}_1 \alpha$ . The coefficients  $e$  and  $s$ , and the energy of normal mode i. e., energy of elementary excitation  $\tilde{\varepsilon}_1$  should coincide with the equations (2-6) and (2-10) respectively, which we shall show now. Above requirement gives the following equation,

$$\begin{aligned} (\varepsilon_1 - \tilde{\varepsilon}_1)e + \gamma s &= 0 \\ \gamma e + (\varepsilon_2 + \tilde{\varepsilon}_1)s &= 0. \end{aligned} \quad (2-13)$$

Equations (2-13) should have the nontrivial solution for  $e$  and  $s$ , so we obtain the following secular equation for  $\tilde{\varepsilon}_1$ ,

$$\begin{vmatrix} \varepsilon_1 - \tilde{\varepsilon}_1, & \gamma \\ \gamma, & \varepsilon_2 + \tilde{\varepsilon}_1 \end{vmatrix} = 0, \quad (2-14)$$

which can be solved as,

$$\tilde{\varepsilon}_1 = \frac{1}{2} (\varepsilon_1 - \varepsilon_2) \pm \sqrt{\varepsilon^2 - \gamma^2}. \quad (2-14')$$

The upper sign gives the same result as that for the equation (2-10). In the limiting case with vanishing  $\gamma$ , this tends to  $\varepsilon_1$  correctly. Then the coefficients  $e$  and  $s$  are determined from the equations (2-13) with substitution (2-10) into  $\tilde{\varepsilon}_1$ , which can be shown to be identical to the equations (2-6) if they are normalized by the equation (2-4). The lower sign corresponds to another normal mode,  $\beta^+ = -sa + eb^+$ , thus for the solution  $\frac{1}{2} (\varepsilon_1 - \varepsilon_2) - \sqrt{\varepsilon^2 - \gamma^2}$  we should put it equal to  $-\tilde{\varepsilon}_2$ . Of course this can be obtained directly from the requirement,  $\beta^+ = eb^+ - sa$  should satisfy the condition of normal coordinate, that is,

$$[\beta^+, \mathcal{H}^{II}] = -\tilde{\varepsilon}_2 \beta^+,$$

which gives the following secular equation for  $\beta^+$  and  $\tilde{\varepsilon}_2$ ,

$$\begin{aligned} (\varepsilon_2 - \tilde{\varepsilon}_2)e + \gamma s &= 0 \\ \gamma e + (\varepsilon_1 + \tilde{\varepsilon}_2)s &= 0 \end{aligned} \quad (2-15)$$

and

$$\begin{vmatrix} \varepsilon_2 - \bar{\varepsilon}_2, & \gamma \\ \gamma, & \varepsilon_1 + \bar{\varepsilon}_2 \end{vmatrix} = 0. \quad (2-16)$$

One of the solutions of the above equations gives exactly the same result as the solution (2-11).

Before proceeding to treat the effects of spin wave interaction, we present here the results of theory of free spin waves in an antiferromagnet. The Hamiltonian is diagonal in the representation of  $\alpha$ 's and  $\beta$ 's,

$$\begin{aligned} \mathcal{H}^{II} = & -2Z|J|S^2N \left\{ 1 + \frac{1}{SN} \sum_{\kappa} (1 - \sqrt{1 - \mathcal{F}_{\kappa}^2}) \right\} \\ & + \sum_{\kappa} \bar{\varepsilon}_1(\kappa) \alpha_{\kappa}^+ \alpha_{\kappa} + \sum_{\kappa} \bar{\varepsilon}_2(\kappa) \beta_{\kappa}^+ \beta_{\kappa}, \end{aligned} \quad (2-17)$$

where

$$\bar{\varepsilon}_1(\varepsilon) = 2Z|J|S\sqrt{1 - \mathcal{F}_{\varepsilon}^2} + g\mu_B H \quad (2-18)$$

and

$$\bar{\varepsilon}_2(\kappa) = 2Z|J|S\sqrt{1 - \mathcal{F}_{\kappa}^2} - g\mu_B H. \quad (2-18')$$

Equations (2-18) and (2-18') give the energies of free spin wave quantum independent on temperature. They are proportional to wave number  $\kappa$  for long wave length like acoustic phonons in contrast with the  $\kappa^2$ -proportionality for magnons in a ferromagnet. This satisfies the requirement of rotational invariance of the problem. The second term in the bracket { } in the equation (2-17) represents the correction to the ground state energy. This gives the measure of deviation of the ground state from the Néel state. The numerical value has been computed by P.W. Anderson<sup>5)</sup> for a simple cubic lattice,

$$\frac{1}{N} \sum_{\kappa} (1 - \sqrt{1 - \mathcal{F}_{\kappa}^2}) = 0.097. \quad (2-19)$$

Another interesting quantity is the reduction of the average  $z$ -component of spins from their saturated magnitude  $S$  in the Néel state.

$$\begin{aligned} \langle \delta S_i^z \rangle &= \frac{1}{N} \sum_i (S - \langle S_i^z \rangle) = \frac{1}{N} \sum_i \langle a_i^+ a_i \rangle \\ &= \frac{1}{N} \sum_{\kappa} \langle a_{\kappa}^+ a_{\kappa} \rangle \end{aligned} \quad (2-20)$$

This can be expressed in terms of variables  $\alpha$ 's and  $\beta$ 's together with the coefficients given by the equations (2-6).

$$\langle \delta S_i^z \rangle = \frac{1}{N} \sum_{\kappa} s_{\kappa}^2 + \frac{1}{N} \sum_{\kappa} e_{\kappa}^2 \langle \alpha_{\kappa}^+ \alpha_{\kappa} \rangle + \frac{1}{N} \sum_{\kappa} s_{\kappa}^2 \langle \beta_{\kappa}^+ \beta_{\kappa} \rangle \quad (2-21)$$

The first term in the equation (2-21) is the reduction of  $z$ -component of spins

which remains at  $T=0^\circ\text{K}$ . We denote this with  $\Delta S$ ,

$$\Delta S = \frac{1}{N} \sum_{\epsilon} s_{\epsilon}^2 = \frac{1}{N} \sum_{\epsilon} \frac{1}{2} \left( \frac{1}{\sqrt{1-\mathcal{F}_{\epsilon}^2}} - 1 \right) = 0.078 \quad (2-22)$$

for a simple cubic lattice.<sup>5)</sup> The second and third terms in the equation (2-21) give the variation of sublattice magnetization with temperature, because in thermal equilibrium  $\langle \alpha_{\epsilon}^+ \alpha_{\epsilon} \rangle$  and  $\langle \beta_{\epsilon}^+ \beta_{\epsilon} \rangle$  are given by the distribution function for Bosons,

$$\langle \alpha_{\epsilon}^+ \alpha_{\epsilon} \rangle = \left\{ \exp \left( \frac{\tilde{\epsilon}_1(\kappa)}{kT} \right) - 1 \right\}^{-1}$$

and

$$\langle \beta_{\epsilon}^+ \beta_{\epsilon} \rangle = \left\{ \exp \left( \frac{\tilde{\epsilon}_2(\kappa)}{kT} \right) - 1 \right\}^{-1}. \quad (2-23)$$

When the external field  $H$  vanishes, both  $\tilde{\epsilon}_1(\kappa)$  and  $\tilde{\epsilon}_2(\kappa)$  coincide with  $\tilde{\epsilon}(\kappa)$  given by

$$\tilde{\epsilon}(\kappa) = 2z |J| S \sqrt{1-\mathcal{F}_{\kappa}^2}. \quad (2-24)$$

This degeneracy reflects the equivalence property of  $A$ - and  $B$ - sublattices to each other in zero applied magnetic fields.

Explicit calculation of  $\langle \delta S_i^z \rangle$  including the temperature variation is straight forward. We can put the sum over wave number vectors  $\kappa$  into the integral

$$\frac{1}{N} \sum_{\kappa} \longrightarrow \frac{1}{(2\pi)^3} \int_{\alpha\kappa=-\pi}^{\alpha\kappa=\pi} \int \int d^3(\alpha\kappa),$$

and further in low temperature we can perform the integration easily with the use of expansion for small  $\kappa$ , because we have the factor  $\exp \left( \frac{\tilde{\epsilon}(\kappa)}{kT} \right)$  in denominator and the trouble of integration-limits disappears for temperature dependent terms. Thus we get the following expression in zero applied magnetic field for a simple cubic lattice,

$$\begin{aligned} \langle \delta S_i^z \rangle = & \Delta S + \frac{2}{\sqrt{3}} \zeta(2) \tau^2 + \frac{16}{3\sqrt{3}} \pi^2 \zeta(4) \tau^4 + \\ & + \frac{416}{9\sqrt{3}} \pi^4 \zeta(6) \tau^6 + \dots, \end{aligned} \quad (2-25)$$

where we used the abbreviation,

$$\tau = kT / (8\pi |J| S) \quad (2-26)$$

and

$$\zeta(p) = \sum_{n=1}^{\infty} \frac{1}{n^p}. \quad (2-27)$$



### III. Effects of spin wave interaction

We proceed to treat our Hamiltonian (1-6) including the interaction terms between spin waves. Our approach goes along the method of equation of motion previously described. Taking the commutator of  $a_\kappa$  with our Hamiltonian (1-6) we obtain,

$$\begin{aligned}
[a_\kappa, \mathcal{H}] &= (g\mu_B H + 2z |J| S) a_\kappa + 2z |J| S b_{\kappa'}^+ \\
&\quad - \frac{1}{N} z |J| \sum_{\kappa_2, \kappa_3, \kappa_4} \delta(\kappa - \kappa_2 - \kappa_3 + \kappa_4) \{ \mathcal{F}_{\kappa_4} a_{\kappa_2} a_{\kappa_3} b_{\kappa_4} + \mathcal{F}_{\kappa_4} b_{\kappa_2}^+ b_{\kappa_3}^+ b_{\kappa_4} \\
&\quad + 2 \mathcal{F}_{\kappa_3 - \kappa_4} a_{\kappa_2} b_{\kappa_3}^+ b_{\kappa_4} \}. \tag{3-1}
\end{aligned}$$

The first and second terms come from the second order part of the Hamiltonian. The last term which is third order in Boson operators represent the effects of mutual interaction between spin waves. These third order terms may have real third order effects which can not be taken into account by the self-consistent averaging procedure. In low temperature region, however, we expect that these real third order processes may be neglected. Thus we replace the quadratic part in Boson operators with the mean value taken at thermal equilibrium.

$$\begin{aligned}
a_{\kappa_2} a_{\kappa_3} b_{\kappa_4} &\longrightarrow a_{\kappa_2} \langle a_{\kappa_3} b_{\kappa_3} \rangle \delta_{\kappa_3, \kappa_4} + a_{\kappa_3} \langle a_{\kappa_2} b_{\kappa_2} \rangle \delta_{\kappa_2, \kappa_4} \\
b_{\kappa_2}^+ b_{\kappa_3}^+ b_{\kappa_4} &\longrightarrow b_{\kappa_2}^+ \langle b_{\kappa_3}^+ b_{\kappa_3} \rangle \delta_{\kappa_3, \kappa_4} + b_{\kappa_3}^+ \langle b_{\kappa_2}^+ b_{\kappa_2} \rangle \delta_{\kappa_2, \kappa_4} \\
a_{\kappa_2} b_{\kappa_3}^+ b_{\kappa_4} &\longrightarrow a_{\kappa_2} \langle b_{\kappa_3}^+ b_{\kappa_3} \rangle \delta_{\kappa_3, \kappa_4} + b_{\kappa_3} \langle a_{\kappa_2} b_{\kappa_2} \rangle \delta_{\kappa_2, \kappa_4} \tag{3-2}
\end{aligned}$$

In this procedure, we neglect the terms such as  $\langle a_\kappa a_{\kappa'} \rangle$ ,  $\langle b_\kappa b_{\kappa'} \rangle$  and  $\langle a_\kappa b_{\kappa'}^+ \rangle$  from the above mentioned view-point. The terms  $\langle a_\kappa b_\kappa \rangle$  and  $\langle a_\kappa^+ b_{\kappa'}^+ \rangle$  in addition to such terms as  $\langle a_\kappa^+ a_\kappa \rangle$  and  $\langle b_\kappa^+ b_\kappa \rangle$  have to be included in the theory, because the normal modes which we seek are expressible in the linear combination of  $a_\kappa$  and  $b_{\kappa'}^+$ . Thus we get the approximate equation of motion for  $a_\kappa$ ,

$$[a_\kappa, \mathcal{H}] = E_1(\kappa) a_\kappa + \Gamma_1(\kappa) b_{\kappa'}^+ \tag{3-3}$$

where

$$E_1(\kappa) = \varepsilon_1(\kappa) - 2z |J| \frac{1}{N} \sum_{\lambda} (\langle b_\lambda^+ b_\lambda \rangle + \langle a_\lambda b_\lambda \rangle \mathcal{F}_\lambda), \tag{3-4}$$

and

$$\Gamma_1(\kappa) = \gamma(\kappa) - 2z |J| \frac{1}{N} \sum_{\lambda} \left( \langle b_\lambda^+ b_\lambda \rangle + \langle a_\lambda b_\lambda \rangle \frac{\mathcal{F}_{\kappa-\lambda}}{\mathcal{F}_\kappa} \right) \mathcal{F}_\kappa. \tag{3-5}$$

In a similar way, we can obtain the equation of motion for  $b_{\kappa'}^+$ ,

$$\begin{aligned}
[b_{\kappa'}^+, \mathcal{H}] &= (g\mu_B H - 2z |J| S) b_{\kappa'}^+ - 2z |J| S a_\kappa \\
&\quad + \frac{1}{N} z |J| \sum_{\kappa_1, \kappa_2, \kappa_3} \delta(\kappa_1 - \kappa_2 - \kappa_3 + \kappa) \{ \mathcal{F}_{\kappa_1} a_{\kappa_1}^+ a_{\kappa_2} a_{\kappa_3} + \mathcal{F}_{\kappa_1} a_{\kappa_1}^+ b_{\kappa_2}^+ b_{\kappa_3}^+ \\
&\quad + 2 \mathcal{F}_{\kappa_3 - \kappa} a_{\kappa_1}^+ a_{\kappa_2} b_{\kappa_3}^+ \}. \tag{3-6}
\end{aligned}$$

The third order terms in this equation are replaced by the following expressions.

$$\begin{aligned}
a_{\epsilon_1}^+ a_{\epsilon_2} a_{\epsilon_3} &\rightarrow a_{\epsilon_2} \langle a_{\epsilon_1}^+ a_{\epsilon_1} \rangle \delta_{\epsilon_1, \epsilon_3} + a_{\epsilon_3} \langle a_{\epsilon_1}^+ a_{\epsilon_1} \rangle \delta_{\epsilon_1, \epsilon_2} \\
a_{\epsilon_1}^+ b_{\epsilon_2}^+ b_{\epsilon_3}^+ &\rightarrow b_{\epsilon_2}^+ \langle a_{\epsilon_1}^+ b_{\epsilon_1}^+ \rangle \delta_{\epsilon_1, \epsilon_3} + b_{\epsilon_3}^+ \langle a_{\epsilon_1}^+ b_{\epsilon_1}^+ \rangle \delta_{\epsilon_1, \epsilon_2} \\
a_{\epsilon_1}^+ a_{\epsilon_2} b_{\epsilon_3}^+ &\rightarrow a_{\epsilon_2} \langle a_{\epsilon_1}^+ b_{\epsilon_1}^+ \rangle \delta_{\epsilon_1, \epsilon_3} + b_{\epsilon_3}^+ \langle a_{\epsilon_1}^+ a_{\epsilon_1} \rangle \delta_{\epsilon_1, \epsilon_2}
\end{aligned} \tag{3-2'}$$

Thus the equation (3-6) may be approximated by

$$[b_{\epsilon}^+, \mathcal{H}] = -\Gamma_2(\kappa) a_{\epsilon} - E_2(\kappa) b_{\epsilon}^+, \tag{3-7}$$

where

$$E_2(\kappa) = \varepsilon_2(\kappa) - 2z|J| \frac{1}{N} \sum_i (\langle a_i^+ a_i \rangle + \langle a_i^+ b_i^+ \rangle \mathcal{F}_i) \tag{3-8}$$

and

$$\Gamma_2(\kappa) = \gamma(\kappa) - 2z|J| \frac{1}{N} \sum_i (\langle a_i^+ a_i \rangle + \langle a_i^+ b_i^+ \rangle \frac{\mathcal{F}_{i-\epsilon}}{\mathcal{F}_i}) \mathcal{F}_{\epsilon}. \tag{3-9}$$

From the equations (3-3) and (3-7), we can determine the energy of spin waves taking into account the effect of mutual interactions self-consistently. In the following we consider the energy of spin waves in zero external magnetic field for simplicity. We may expect

$$\langle a_i^+ a_i \rangle = \langle b_i^+ b_i \rangle \tag{3-10}$$

and

$$\langle a_i b_i \rangle = \langle a_i^+ b_i^+ \rangle \tag{3-11}$$

from the consideration of the equivalence of  $A$ - and  $B$ -sublattices, in zero magnetic field and the properties of transformations (2-3). Further in performing the  $\lambda$ -summation in the equations (3-5) and (3-9),  $\mathcal{F}_{\epsilon-\lambda}$  may be decomposed into  $\mathcal{F}_{\epsilon} \mathcal{F}_{\lambda}$  from the consideration of crystal symmetry. Thus we may have

$$E_1(\kappa) = E_2(\kappa) \rightarrow E(\kappa) = \varepsilon(\kappa) (1 + \mathcal{D}) \tag{3-12}$$

and

$$\Gamma_1(\kappa) = \Gamma_2(\kappa) \rightarrow \Gamma(\kappa) = \gamma(\kappa) (1 + \mathcal{D}) \tag{3-12}$$

where

$$\mathcal{D} = -\frac{1}{NS} \sum_i (\langle a_i^+ a_i \rangle + \mathcal{F}_i \langle a_i b_i \rangle). \tag{3-14}$$

The secular equation for  $\tilde{E}(\kappa)$  i.e., the spin wave energy which contains the effects of mutual interactions is expressed as follows,

$$\begin{aligned}
(E(\kappa) - \tilde{E}(\kappa)) e'_{\epsilon} + \Gamma(\kappa) s'_{\epsilon} &= 0 \\
\Gamma(\kappa) e'_{\epsilon} + (E(\kappa) + \tilde{E}(\kappa)) s'_{\epsilon} &= 0.
\end{aligned} \tag{3-15}$$

The solution for the equation (3-15) is obtained with use of  $\tilde{\varepsilon}(\kappa)$ ,

$$\tilde{E}(\kappa) = \tilde{\varepsilon}(\kappa) (1 + \mathcal{D}) \tag{3-16}$$

where the effects of mutual interaction is condensed into the factor  $(1 + \mathcal{D})$ . We notice, however, the mixing coefficients in  $\alpha$ - (or  $\beta^+$ -) mode are identical with those obtained in the paragraph II. This means that the new normal mode  $\alpha'_{\epsilon}$  remains

invariant and equal to  $\alpha_r$  in free spin waves, whereas their energy  $\tilde{E}(\kappa)$  undergoes the change due to the effects of mutual interaction. The factor  $\Delta$  is expressed in terms of the above-mentioned normal coordinates, i.e., the mixing coefficients  $e_r$  and  $s_r$ , and with the distribution function for Bosons,  $N_r$ .

$$\Delta = \Delta_0 - \frac{1}{NS} \sum N_r (e_r^2 + s_r^2 + 2\mathcal{F}_r e_r s_r) \quad (3-17)$$

We denote here with  $\Delta_0$  the temperature independent part in  $\Delta$ , that is, the part due to the interaction effects in the ground state.

$$\begin{aligned} \Delta_0 &= -\frac{1}{NS} \sum_r (s_r^2 + \mathcal{F}_r e_r s_r) \\ &= \frac{1}{2NS} \sum_r \left(1 - \sqrt{1 - \mathcal{F}_r^2}\right) = \frac{1}{2S} \times 0.097 \quad (\text{for a simple cubic lattice}) \end{aligned} \quad (3-18)$$

The second term in  $\Delta$  is expressed in terms of the renormalized Boson distribution function  $N_r$  with the new energy  $\tilde{E}(\kappa)$ .

$$\Delta = \Delta_0 - \frac{1}{NS} \sum N_r \sqrt{1 - \mathcal{F}_r^2} \quad (3-19)$$

and

$$N_r = \left\{ \exp\left(\frac{\tilde{E}(\kappa)}{kT}\right) - 1 \right\}^{-1} \quad (3-20)$$

The sum over the wave number vector  $\kappa$  in the equation (3-19) is carried out in a similar way done in the paragraph II for  $\langle \delta S_i^z \rangle$ . Thus we get

$$\begin{aligned} \Delta &= \Delta_0 - \frac{1}{S} \left[ \frac{16}{3\sqrt{3}} \pi^2 \zeta(4) \frac{\tau^4}{(1+\Delta)^4} + \frac{1280}{27\sqrt{3}} \pi^4 \zeta(6) \frac{\tau^6}{(1+\Delta)^6} \right. \\ &\quad \left. + \frac{23296}{27\sqrt{3}} \pi^6 \zeta(8) \frac{\tau^8}{(1+\Delta)^8} + \dots \right], \end{aligned}$$

which can be solved with the use of successive approximation.

$$\begin{aligned} \Delta &= \Delta_0 - \frac{1}{S} \left[ \frac{16}{3\sqrt{3}} \pi^2 \zeta(4) \frac{\tau^4}{(1+\Delta_0)^4} + \frac{1280}{27\sqrt{3}} \pi^4 \zeta(6) \frac{\tau^6}{(1+\Delta_0)^6} \right. \\ &\quad \left. + \left\{ \frac{23296}{27\sqrt{3}} \pi^6 \zeta(8) + \frac{1024}{27S} \pi^4 \zeta^2(4) \frac{1}{(1+\Delta_0)} \right\} \frac{\tau^8}{(1+\Delta_0)^8} + \dots \right] \end{aligned} \quad (3-21)$$

For the reduction of the magnitude of the sublattice magnetization the influence of mutual interaction makes a contribution through the effects of renormalization of spin wave energies, but  $\Delta S$  given by the equation (2-22) is not modified because of the independence on temperature of the normal mode coefficients,

$$\begin{aligned} \langle \delta S_i^z \rangle &= \Delta S + \left[ \frac{2}{\sqrt{3}} \zeta(2) \frac{\tau^2}{(1+\Delta)^2} + \frac{16}{3\sqrt{3}} \pi^2 \zeta(4) \frac{\tau^4}{(1+\Delta)^4} \right. \\ &\quad \left. + \frac{416}{9\sqrt{3}} \pi^4 \zeta(6) \frac{\tau^6}{(1+\Delta)^6} + \dots \right], \end{aligned}$$

which is solved using the result (3-21),

$$\begin{aligned} \langle \delta S_{i^z} \rangle = & 4S + \left[ \frac{2}{\sqrt{3}} \zeta(2) \frac{\tau^2}{(1+\mathcal{A}_0)^2} + \frac{16}{3\sqrt{3}} \pi^2 \zeta(4) \frac{\tau^4}{(1+\mathcal{A}_0)^4} \right. \\ & \left. + \left( \frac{416}{9\sqrt{3}} \pi^4 \zeta(6) + \frac{64}{9S} \pi^2 \zeta(2) \zeta(4) \frac{1}{1+\mathcal{A}_0} \right) \frac{\tau^6}{(1+\mathcal{A}_0)^6} + \dots \right]. \quad (3-22) \end{aligned}$$

## VI. Discussions and conclusion

We have investigated the effects of mutual interaction between spin waves for the energy of elementary excitation and the reduction of sublattice magnetization by an approach along the self-consistent linearization for the equation of motion.

We compare the spin wave energy (3-16) in which  $\mathcal{A}$  is expressed by the equations (3-18) and (3-21) with the corresponding one (2-24). We see that  $\tilde{\varepsilon}(\kappa)$  is larger than  $\varepsilon(\kappa)$  by the factor  $(1+\mathcal{A}_0)$  at  $0^\circ\text{K}$ , and both of them are proportional to the magnitude of wave vector  $\kappa$  for long wave-length magnons. The factor  $(1+\mathcal{A}_0)$  means the improvement achieved with the introduction of mutual interaction in the ground state for the velocity of magnons. This seems to be along the right direction for an antiferromagnet in a three dimensional lattice, although we have an exact solution only for a linear chain problem.<sup>6)</sup> In this one dimensional problem the exact theory gives the larger magnon velocity than that in P. W. Anderson's theory. The temperature dependence of spin wave energy is seen to appear in the leading term proportional to  $T^4$ . We compare this temperature dependence with the  $T^2$ -dependence which is obtained by the approximation due to Tyablikov-decoupling in the Green function theory.<sup>7)</sup> The method of Tyablikov-decoupling has the merit that the behaviour in wider temperature range is well approximated but we notice that the temperature dependence for the excitation energy is a qualitative one, as we see for a Heisenberg ferromagnet in our previous work.<sup>2)</sup> We expect that we may obtain the knowledge about the life time of spin wave quantum when we take into account higher order effects which are not contained in our approximation and are neglected in the present treatment.

Next, the equation (3-22) should be compared with the corresponding one, namely the equation (2-25) for the reduction of sublattice magnetization. We notice  $4S$  is not modified by mutual interactions between spin waves. This is due to the fact that the coefficients of the Bogolyubov-transformation are identical with those without interactions in our approximation. The normal modes in free spin wave theory have rather unexpected sound basis. The origin of the temperature variation of their energies does not consist in the change of their own character but consists in the change of the environment into which magnons are created and in the variation of the mutual interaction which magnons feel. The modification is introduced through the renormalization of spin wave energies. These effects are seen to be the replacement of  $\tau$  in the equation (2-25) by  $\tau/(1+\mathcal{A}_0)$  and further the modifications in

the coefficients in  $\tau$  appear for terms higher than  $\tau^6$ -terms. We cite here the corresponding expression due to the method of Tyablikov-decoupling approximation,

$$\langle \delta S_i^z \rangle_{Tyab.} = 4S + \left[ \frac{2}{\sqrt{3}} \zeta(2) \tau^2 + \left( \frac{16}{3\sqrt{3}} \pi^2 \zeta(4) + \frac{16}{3} \zeta^2(2) \right) \tau^4 + \dots \right],$$

and that for the energy of elementary excitation which has the  $T^2$ -dependence,

$$\tilde{E}(\kappa)_{Tyab.} = 2z|J|S\sqrt{1-\mathcal{F}^2} (1 - 2\langle \delta S_i^z \rangle).$$

Our approximation represented by the replacements (3-2) and (3-2') corresponds to Hartree-Fock type decoupling approximation in the Green function theory.<sup>2)</sup> In the Green function theory, we set up the equation of motion for the Green function to get the new higher order Green function, which are expressed with the decoupling approximation introducing the statistical parameter. We determine this statistical parameter with the requirement of self-consistency. We have used the equation of motion approach in order to gain the insight for the wave function as well as the energy of elementary excitation, because in the Green function theory we devote our attention to the elementary excitation energies only.

Finally we shall mention briefly the effect of externally applied field. In real crystals we have to consider the effects of anisotropic fields in addition to the applied field. If they are not included properly in the expression for  $\tilde{E}(\kappa)$ , we may obtain the negative spin wave energies for some values of  $\kappa$ . This represents the problem of instability, which we do not consider at present.

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